ANNUAL REPORT

TO

THE OFFICE OF NAVAL RESEARCH
ARLINGTON, VA 22217

FOR

SOLID-STATE DYNAMICS AND QUANTUM TRANSPORT IN NOVEL SEMICONDUCTOR NANOSTRUCTURES

ONR Grant No: N00014-90-J-1835
R&T Project Code: 314x001---01
NCSU FAS No: 5-31132

Submitted by

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For the Period October 1, 1993 - September 30, 1994

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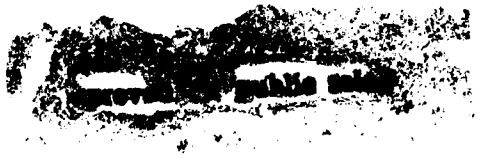

SUBMITTED OCTOBER 1994

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1. PROJECT SUMMARY

The objective of this research program is to study theoretically the underlying principles of solid-state dynamics and quantum mechanical transport of carriers in ultrasmall novel semiconductor devices. The areas of research are: 1) theory of phonon modes in reduced dimensions, 2) effects of band structure on electronic and optical properties of heterostructures, and 3) quantum transport in solids with special emphasis on the non-perturbative role of high-electric fields and many-body effects in dynamical processes. The treatment of these problems is mainly analytical through the development of macroscopic and microscopic physical models with an emphasis on quantum mechanical principles. At the same time, numerical approaches has also been utilized for realistic solutions with accuracy. Specific subjects discussed in this report include the effects of confinement and localization on optical and acoustic phonon modes, band mixing in phonon-assisted transitions, and Bloch electron quantum transport theory under hot-electron conditions. The knowledge developed in this work will be of major importance in explaining the novel phenomena and fundamental questions relating to the breakdown of classical solid-state electronics as device dimensional scales are reduced to the submicron and ultra-submicron regime.

2. PROJECT DESCRIPTION

2.1 Introduction

Recent advances in semiconductor materials growth techniques, such as molecular beam epitaxy (MBE), metalorganic chemical vapor deposition (MOCVD), and atomic layer epitaxy (ALE), have made possible the fabrication of devices with one or more dimensions approaching the spacing between planes of atoms. These nanometer-scale techniques have also opened new possibilities for "band gap engineering" of novel semiconductor devices, including heterostructures with spatially modulated energy band gaps. By using the variability of the boundary conditions which can be imposed on the wave functions, electrical and optical responses in these structures can be tailored virtually at will. As fabrication technology has allowed such ultrasmall structures to be realized, many new and fundamental questions have emerged concerning the underlying physics of small dimensions with complex, quantum-scale boundary conditions in semiconductor devices. Important issues now under investigation include quantum mechanical phenomena such as size quantization, phase coherence, and highly nonequilibrium transport in which a perturbative treatment or the assumption of linear response is not applicable (see, for example, Refs. 1-3). More than ever before, it is important that our ability to analyze these physical phenomena occurring at ultrasmall scales proceeds technological developments and leads the way to future advances.

In 1990, the Office of Naval Research initiated sponsorship of a basic research program in the Department of Electrical and Computer Engineering at North Carolina State University. The general goal of this research program is to study theoretically solid-state dynamics and quantum mechanical transport of carriers in ultrasmall novel semiconductor devices. The emphasis is on the development of physical understanding of the novel phenomena mainly through analytical approaches. However, numerical evaluation will also be employed for realistic solutions with accuracy. Our efforts have been devoted to investigating three important problems. The first one is the theory of phonon modes in

heterostructures. The changes in longitudinal-optical (LO) phonon frequencies, lifetimes, and interactions with carriers as a result of reduced dimensionality are the main subjects in this part of the research. Due to the advent of lattice mismatched strained-layer (i.e., pseudomorphic) structures, the effects of strain on LO-phonon modes have been investigated as well. Recently, the scope of this research effort has been expanded to investigate the effects of acoustic phonon confinement on piezoelectric scattering and deformation potential scattering. The results will be of major importance to a wide variety of nanoscale semiconductor devices in which the scattering by quantized phonon modes plays a significant and, at times, a dominant role in determining the electronic and optoelectronic properties. The second topic is the quantum mechanical transport of charge carriers with specific emphasis on the effects of electron-electron and electron-phonon interactions in the presence of high-electric fields and many-body effects in dynamical processes. A novel formalism for treating Bloch electron dynamics and quantum transport in electric fields of arbitrary strength and time dependence has been studied in an attempt to include all quantum mechanical effects collectively in the lowest order in the scattering strength [1]. Specific interest in this inelastic scattering problem arises from issues and questions relevant to the role of high-electric fields in influencing transport, electron relaxation, and noise generation as well as ionization processes in quantum wells, tunnel barriers, superlattices, and quantum wires. At the same time, attempts have been made to study the effects of quantum mechanical principles on carrier transport with more macroscopic approaches such as dielectric function theory. As the third topic, we have recently begun to emphasize the effects of band structure which are critical to understanding electronic and optoelectronic properties of heterostructures. Detailed knowledge of band structure in the presence of heterointerfaces, such as mixing and evanescent states, is essential for the characteristic response of a mesoscopic system which is beyond the realm of the conventional effective mass approximation. The main subjects of interest in this topic include the effects of band mixing in linear and nonlinear optical constants, tunneling, and phonon-assisted transitions.

Although only four years old, this program has already resulted in thirty nine refereed publications in the literature, five additional manuscripts are currently in press, and one more has been submitted to a major technical journal. Numerous invited talks and presentations have been and will be given at conferences and workshops throughout the United States and in other countries. A listing of these publications is given in Appendix A. In addition, this research program provides a perfect complement to other aspects of our research efforts in which numerical modeling aspects of transport study are emphasized. Due to the complicated geometry and boundary conditions, a realistic model for a realistic device structure is attainable only through numerical approaches. The accurate physical models and understanding developed in this research facilitates the development of the numerical models better able to explain experimental observations and to predict new physical phenomena. Overall, this research program supported by ONR has been efficient and productive. The quality of our program will continue to improve in the future. In this annual report, the progress and accomplishments made during the past contract period will be summarized.

The structure of the rest of this report is as follows: in Section 2.2, the research results of the past contract period are summarized; Section 2.3 provides the list of publications resulting from this research supported by ONR during the 1993-94 contract period; Section 3 contains background information describing project personnel; and the Appendices include a list of refereed publications supported by this research program since 1990 and the title page of each paper published during the 1993-94 contract period.

2.2 Summary of Research Results

This section provides the current status of our research efforts on the theory of electron-acoustic-phonon interactions, the LO phonon lifetime, the effects of band mixing, and quantum mechanical transport in semiconductor nanostructures. The major accomplishments during the past contract period are:

- We have derived appropriately normalized approximate expressions for the acoustic phonons confined in a free-standing rectangular quantum wire by quantizing the acoustic phonon displacements and, subsequently, have formulated the interaction Hamiltonian for the deformation potential associated with confined acoustic phonon modes in rectangular quantum wires. The deformation potential scattering rates due to the confined acoustic phonon modes have been obtained for GaAs quantum wires with a range of cross sectional dimensions. Comparison with the corresponding rates obtained with bulk phonons demonstrates that a proper treatment of confined acoustic phonons may be essential to correctly modeling electron scattering rates at low energies in nanoscale structures.
- We have developed an approach to calculate the lifetime of LO phonons via emission of two acoustic phonons in bulk zincblende semiconductors. The interaction Hamiltonian for anharmonic decay is derived based on Keating's treatment of anharmonic contributions in the elastic strain energy of a crystal. Application of this model to bulk GaAs provides excellent agreement with available experimental data. Since the parameters employed in the model can be obtained experimentally and theoretically, our approach provides a useful tool for investigating LO phonon lifetimes in semiconductors.
- We have calculated the Γ-X intersubband scattering rates due to optical phonon emission by using a tight binding method for electrons and the dielectric continuum model for optical phonons, and have demonstrated that this is an important mechanism for the Γ-X relaxation process in type-II superlattices. Among the various phonon modes, the strongest are found to be the

AlAs confined modes and the weakest are the GaAs confined modes. It is also shown that the parity of electron states affects the transition rates significantly. The theoretical results obtained from our calculations are in general agreement with the experimental data.

- We have developed an extension of the Kronig-Penney model to treat mixings of different valleys in type-II superlattices. The value of the mixing parameter used in this model was deduced by comparison with more sophisticated theory and various experiments for the GaAs/AlAs material system. It is shown that with the use of a single value for the mixing parameter, this simple and efficient model can reasonably reproduce the important aspects of valley mixing effects in GaAs/AlAs superlattices over a wide range of layer thicknesses.
- We have developed a novel formalism for treating Bloch electron dynamics and quantum transport in a superimposed uniform and oscillatory electric field. Based on this treatment, a complete analysis of single-band and multi-band processes and the total transition rates including all possible transitions have been obtained. We have also investigated the effect of localized impurities on transport of an electron in a uniform electric field, and have formulated a theory to describe Bloch electron transport through spatially localized inhomogeneous potential barriers using a field-dependent Green's function approach.

Each of these results is presented in detail in the following discussions.

Electron-confined-acoustic-phonon scattering in quantum wires

A number of proposed applications of mesoscopic electronic structures involve carrier transport at low temperatures and low carrier energies; frequently, the regime of interest is one where dimensional confinement modifies the phase space substantially. It is well known that in this low temperature, low energy regime, acoustic phonons play an enhanced role in carrier scattering and may dominate over the scattering of carriers by optical phonons. In addition, in nanoscale structures it is possible that phase space restrictions may weaken or forbid optical phonon scattering processes that would normally

dominate in bulk structures. Recently, there has been an extensive effort to study the role of dimensional confinement in modifying LO phonon modes and their interactions with charge carriers in nanoscale and mesoscopic semiconductor structures, as demonstrated by numerous publications by us (supported by this program) as well as by others. On the other hand, there are relatively few treatments dealing with the role of dimensional confinement in modifying acoustic phonon modes and their interactions with charge carriers. In spite of the fact that there is an extensive literature on the theory of acoustic modes in conventional waveguides, resonators and related structures, few efforts have been reported to formulate a theory of acoustic phonons in nanoscale structures where both phonon confinement and a quantum mechanical treatment of phonon normalization are essential. The necessity for such theoretical treatments has been demonstrated recently by experimental studies providing both direct and indirect evidence [4,5] of the importance of acoustic phonon confinement in reduced dimensional electronic structures.

During the past contract period, we have initiated a research effort to study the effects of confinement on acoustic phonons and their interactions with electrons in nanoscale structures. As a first project in this area, we have developed appropriately normalized approximate expressions for the acoustic phonons confined in a free-standing rectangular quantum wire by quantizing the acoustic phonon displacements and, subsequently, have formulated the interaction Hamiltonian for the deformation potential associated with confined acoustic phonon modes in rectangular quantum wires. In addition, preliminary works have been done to determine the role of acoustic phonon confinement in modifying piezoelectric scattering as well as deformation potential scattering in a number of different quantum-wire and quantum-dot geometries of significant interest in nanoelectronics and optoelectronics. In this section, we present our study on the effects of confinement on acoustic phonon modes in a free-standing rectangular quantum wire and the associated deformation potential scattering.

The specific structure of our interest is a free-standing rectangular quantum wire of infinite length in the z-direction having an x-directed height (or thickness), 2a, and a y-directed width, 2d; the origin of coordinates in the x-y plane is taken to be at the geometric center of the rectangular cross section. Our approach on confined acoustic phonon modes is based on the classic study by Morse on acoustic modes in a conventional waveguide of rectangular cross section [6]. Through an extended analysis, Morse has derived an approximate set of hybrid compressional, or dilatational, acoustic modes which are found to accurately approximate the experimentally observed modes over a wide range of conditions. Specifically, he has found that the approximate hybrid modes derived by assuming separable boundary conditions have simple analytical representations (as in our previous analysis of optical phonon modes in rectangular quantum wires) and provide convenient approximations for the rectangular geometry when the cross-sectional dimensions have aspect ratios of approximately 2 or greater. Adopting Morse's form for the approximate separation-of-variable solution, the x-, y-, and z-directed acoustic mode displacements for the "thickness" mode may be written, respectively, as

$$u_1 = A\{\sin k_1 x + \alpha \sin k_2 x\}\cos(hy)e^{i\gamma(z-ct)}, \tag{1a}$$

$$v_1 = A\{\frac{h}{k_1}\cos k_1 x + \beta \cos k_2 x\}\sin(hy)e^{i\gamma(z-ct)}, \tag{1b}$$

$$w_1 = iA\{-\frac{\gamma}{k_1}\cos k_1 x + \frac{1}{\gamma}(k_2\alpha + h\beta)\cos k_2 x\}\cos(hy)e^{i\gamma(z-ct)}, \tag{1c}$$

where A is the normalization constant, γ is the z-directed free wavevector, c is the phase velocity, α and β are defined by

$$\alpha = -\frac{\sin k_1 a}{\sin k_2 a}\frac{2(h^2+\gamma^2)}{(\gamma^2+h^2-k_2^2)}, \tag{2a}$$

$$\beta = \frac{\sin k_1 a}{\sin k_2 a}\frac{2k_2 h}{(\gamma^2+h^2-k_2^2)}, \tag{2b}$$

and

$$k_1^2 + h^2 = \gamma^2[(c/c_d)^2 - 1] , \tag{3a}$$

$$k_2^2 + h^2 = \gamma^2[(c/c_s)^2 - 1] , \tag{3b}$$

with the compressional, or dilatational, sound speed, c_d, and the transverse, or shear, sound speed, c_s. The boundary conditions for acoustic modes in free-standing structures require that the stress components normal to the surface vanish at the surface. Application of this condition at $x=\pm a$ (i.e., $T_{xx}=T_{yx}=T_{zx}=0$ at $x=\pm a$) results in an equation which serves as the dispersion relation,

$$\frac{\tan k_2 a}{\tan k_1 a} = -\frac{4k_1k_2(h^2+\gamma^2)}{(h^2+\gamma^2-k_2^2)^2} . \tag{4}$$

However, the corresponding boundary condition at $y=\pm d$ (i.e., $T_{yy}=T_{xy}=T_{zy}=0$) cannot be satisfied exactly due to the well-known difficulties at the corners. When $d \geq 2a$, this problem can be circumvented since the two shear stresses T_{xy} and T_{zy} become negligible. Accordingly, only the extensional stress T_{yy} needs to vanish at the surface; this condition requires,

$$h = (n + \frac{1}{2})\frac{\pi}{d} , \quad n = 0,1,2, \cdots . \tag{5}$$

The principal thickness mode (i.e., $n=0$ or $h=\pi/2d$) has no nodal surfaces parallel to the length, and is the dominant mode. For a given h and γ, both k_1 and k_2 may be written in terms of c as shown in Eq. (3). When substituted in Eq. (4), the phase velocity c has multiple solutions due to the periodic nature of the trigonometric functions. Consequently, the dispersion relation or the phonon frequency ω_γ ($=c\gamma$) in a quantum wire needs an additional index m to distinguish different modes.

In addition to the thickness modes, another set of acoustic modes is observed experimentally [6]. These modes corresponds to "width modes" and are determined in a manner similar to that used to determine the thickness modes. By satisfying the boundary conditions on the stress at $y=\pm d$ (i.e., $T_{yy}=T_{xy}=T_{zy}=0$), the solutions for the width modes show expressions analogous to Eq. (1) with the roles of x and y as well as k and h interchanged, respectively. For these modes, k is then determined

by approximate boundary conditions at x=±a. The dispersion relation for the width mode is identical in form to Eq. (4). As for the thickness modes, the principal mode with k=0 is the dominant mode. Figure 1 depicts the dispersion curves of the six lowest thickness modes ($h=\pi/2d$, m=1, · · · ,6) and the corresponding width modes (k=0, m=1, · · · ,6) for a GaAs quantum wire free-standing in vacuum. The quantum wire cross sectional dimension is chosen to be 28.3 Å by 56.6 Å (i.e., 10 by 20 monolayers). As expected, the width modes tend to have lower energies than the thickness modes since the width is greater than the thickness for the case represented in this figure.

When properly quantized, the acoustic modes derived in conventional waveguides can be applied to describe the characteristics of confined acoustic phonon modes in semiconductor quantum wires. Following the quantization procedure, the normalization constant in Eq. (1) may be determined by

$$\frac{1}{4ad}\int_{-a}^{+a} dx \int_{-d}^{+d} dy \, \{u_l u_l^* + v_l v_l^* + w_l w_l^*\} = \frac{\hbar}{2M\omega_\gamma} , \tag{6}$$

where M is the mass for a unit cell and ω_γ is the frequency corresponding to the mode with wavevector γ in the z direction, as described before. With this condition, the classical phonon displacement may be written in terms of quantized normal coordinates, and the interaction Hamiltonians caused by lattice vibrations can be developed readily. In particular, the interaction Hamiltonian for deformation potential scattering is given by,

$$H_{def} = E_a \nabla \cdot \vec{u}(\vec{r},t) = E_a \sum_{\gamma,n,m} [c_{n,m}(\gamma) + c_{n,m}^{\dagger}(-\gamma)] \left[\frac{\partial u_l}{\partial x} + \frac{\partial v_l}{\partial y} + \frac{\partial w_l}{\partial z} \right] , \tag{7}$$

where $c_{n,m}(\gamma)$ and $c_{n,m}^{\dagger}(-\gamma)$ are the usual annihilation and creation operators. In this equation, the sum over γ represents the usual integration over wavevector, while the sums over n and m represent the addition of the various acoustic phonon modes. When the expressions given in Eqs. (1) and (6) are adopted for determining the phonon displacements, this Hamiltonian provides the desired description for the electron-acoustic-phonon interaction in rectangular quantum wires, and replaces the commonly-

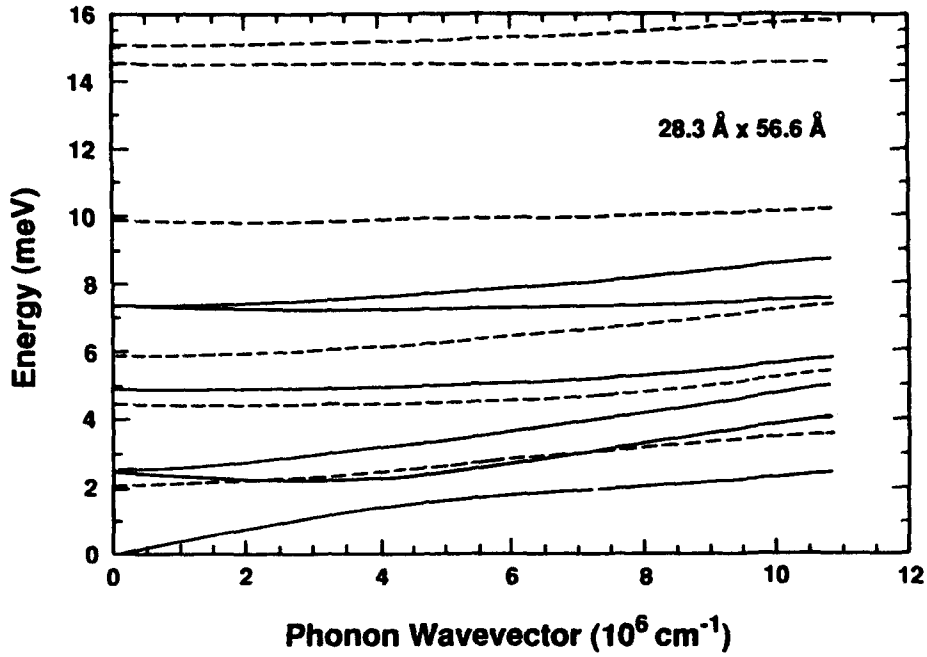

Figure 1. Dispersion curves for the six lowest width and thickness modes (m = 1, · · · ,6) of a 28.3 Å × 56.6 Å GaAs quantum wire. The solid lines are for the width modes, and the dashed lines are for the thickness modes.

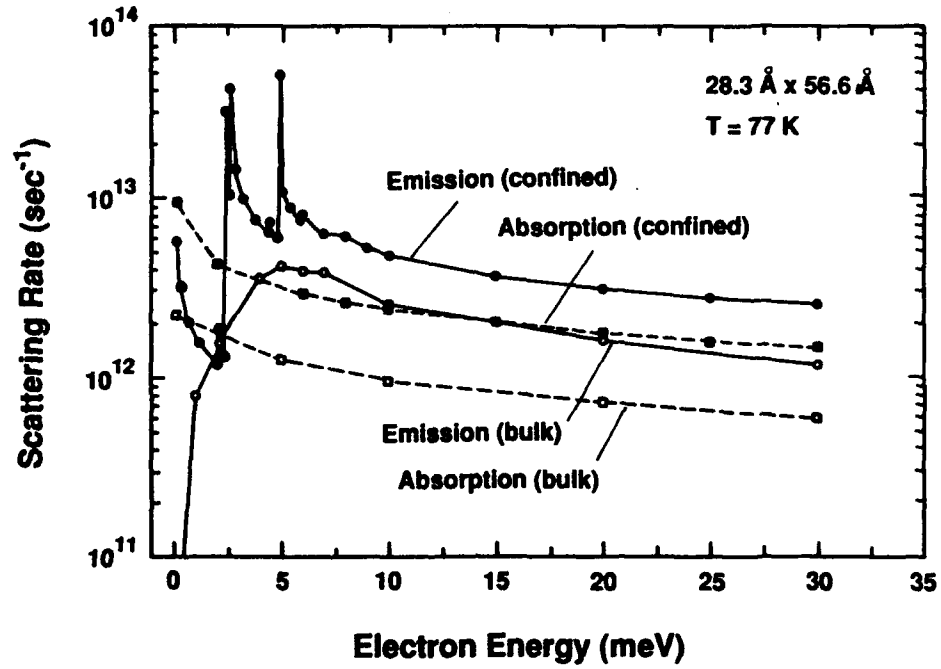

Figure 2. Deformation potential scattering rates for bulk and confined acoustic phonon modes in a 28.3 Å × 56.6 Å GaAs quantum wire at 77 K. Enhancements in the scattering rates for the case of confined acoustic modes occur at the onset of emission for the various width and thickness modes. These thresholds are at 0.03, 2.36, 2.55, 4.90, 7.30, and 7.40 meV for the width modes, and at 2.06, 4.44, 5.90, 9.87, 14.5, and 15.1 meV for the thickness modes. The plotting resolution depicted is not fine enough to illustrate fully the importance of the density-of-states effects in the rectangular quantum wire.

used Hamiltonian based on bulk acoustic phonons.

Based on the deformation potential interaction Hamiltonian derived above, we have calculated the electron-acoustic-phonon scattering rates in a GaAs rectangular quantum wire free-standing in vacuum. For simplicity, an isotropic cubic medium has been assumed and the compressional, or longitudinal, sound speed has been taken to be that of GaAs; it should be noted that imposing both of these constraints makes it impossible to have a transverse sound speed matching that of GaAs. This is a consequence of the fact that GaAs may be treated as having an isotropic elastic tension only in a very rough approximation. In this work, Poisson's ratio, σ, is taken to have the physically reasonable value of 1/3; this choice fixes the value of c_s for a given c_d in Eq. (3). The Fermi Golden Rule scattering rates for emission and absorption are plotted in Fig. 2 as functions of electron energy. In this figure, the extreme quantum limit is assumed and the rates are obtained for the ground (electronic) states at 77 K. For comparison, the results for bulk acoustic modes are shown as well. Two distinct and important features are obvious from Fig. 2. First, the appearance of structure is prominent in the scattering rates (for confined phonons) which results from the energy threshold for the different mode values, m, of the thickness and width modes. As can be seen from Fig. 2, each of these modes makes a notable contribution to the density-of-states and to the scattering rate. In particular, the scattering rates at low energies show pronounced peaks and are strongly enhanced due to the dominance of selected compressional modes in the emission process. Thus, it is essential to retain a number of acoustic modes for an accurate estimation of scattering rates. The results shown in Fig. 2 have been obtained by including the six lowest-order thickness modes as well as the six lowest-order width modes. Due to the limited resolution in plotting, the details of the one dimensional nature (such as the number of peaks and their heights) are not illustrated fully in this figure. The second important feature of Fig. 2 is that the scattering rates for the case of the confined acoustic modes are higher than the corresponding scattering rates based on bulk phonons. These enhanced scattering rates provide an indication that conceptual designs for mesoscopic devices need to be based on an awareness of the fact that confined acoustic

modes may play a significant role in carrier transport in these devices. It is also important to note that the sets of the solutions for confined acoustic modes given above (i.e., thickness and width modes) may not be complete. Thus it is plausible that confinement may enhance the electron-acoustic-phonon scattering rate even more than it is presented in this work.

Theoretical calculation of LO phonon lifetimes

In polar semiconductors, carrier energy and momentum relaxation processes are frequently dominated by the interaction of carriers with optical phonons, particularly the LO phonons. It is now well-known that carrier relaxation rates underlie a range of phenomena other than simple carrier transport. Previous analyses of carrier relaxation in semiconductor microstructures have demonstrated that emission alone does not, in general, dominate the carrier energy loss rates since subsequent optical phonon absorption events slow the relaxation process. Instead, it has been shown that the overall carrier relaxation rate is frequently dominated by the decay of the strongly interacting optical phonon into weakly interacting acoustic phonons. Thus, the detailed knowledge of optical phonon decay, which is characterized by lifetime, is of major importance in understanding carrier dynamics in semiconductors. The decay process of optical phonons arises primarily from the three-phonon interaction through the anharmonic terms of the crystal potential energy. This phenomenon has been scrutinized by a number of authors mostly in bulk materials [7-12]. The approaches taken by these authors can be classified broadly in two categories: highly complex and complete microscopic models [7,8,11] with parameters which are very difficult to measure, and simpler macroscopic treatments [9,10] where attempts have been made to approximate various anharmonic contributions by replacing them with a single parameter related to an average of third order elastic constants or a Grüneisen constant. An approach similar to the latter treatments has been adopted recently to estimate optical phonon lifetimes in quantum wells by taking into account the envelope functions of the confined optical phonons [12]. A major difficulty associated with the simple approaches is that they rely on finding a valid expression for this *appropri-*

ately averaged single parameter from the experimentally measurable quantities. Otherwise, it simply acts as a fitting parameter without a solid physical basis.

Last year, we began an investigation on anharmonic decay of LO phonons in nanostructures. The principal aim of this effort is to study the effects of reduced dimensions on the LO phonon lifetime and the resulting carrier relaxation processes through the development of a physically valid model. To facilitate the capability to *predict*, the sought-after model must incorporate parameters based on a firm physical footing, which can be either measured experimentally or estimated from other theoretical analyses. Such a model without fitting parameters has not yet been formulated even in bulk materials not to mention in heterostructures. As a first step toward this goal, we have developed an approach to calculate the lifetime of LO phonons via emission of two acoustic phonons in bulk zincblende semiconductors. The interaction Hamiltonian for anharmonic decay is derived based on Keating's treatment of anharmonic contributions in the elastic strain energy of a crystal [13]. Application of this model to bulk GaAs provides excellent agreement with available experimental data. Since the parameters employed in the model can be obtained experimentally and theoretically, our approach provides a useful tool to investigate LO phonon lifetimes in semiconductors. A brief summary of the formalism and results of our calculations are provided below.

When a crystal potential is expanded in powers of displacements of the atoms from their equilibrium positions, we obtain a quadratic term along with cubic, quartic and other higher order terms. For simple analysis of the dispersion relation, it is acceptable to consider only the quadratic term and ignore the rest of the higher order terms in what is known as the harmonic approximation. However, the harmonic approach cannot describe the decay of phonon modes caused by the cubic and other higher-order terms, also known as the anharmonic terms, in the crystal potential. It is generally accepted that the cubic term dominates over all anharmonic terms in phonon decay. For this process involving three phonons, the interaction Hamiltonian may be written as

$$H_{\vec{k}j;\vec{k}'j';\vec{k}''j''} = \frac{1}{\sqrt{N}} P(\vec{k}j;\vec{k}'j';\vec{k}''j'')\, u_{\vec{k}j} u_{\vec{k}'j'} u_{\vec{k}''j''} , \tag{8}$$

where $\vec{k}$, $\vec{k}'$, and $\vec{k}''$ (j, j', and j'') represent the phonon wavevectors (polarization modes), N is the number of unit cells, and P describes the cubic coupling. The displacement for the phonon mode in normal coordinates may be represented as

$$u_{\vec{k}j} = \left[\frac{\hbar}{2m\omega_{\vec{k}j}}\right]^{1/2} e_{\vec{k}j} \left(a_{\vec{k}j} e^{i\vec{k}\cdot\vec{r}} + a^{\dagger}_{\vec{k}j} e^{-i\vec{k}\cdot\vec{r}}\right) , \tag{9}$$

where $a_{\vec{k}j}$ and $a^{\dagger}_{\vec{k}j}$ are the annihilation and creation operators, $e_{\vec{k}j}$ is the polarization vector, m is the average mass of the lattice atoms, and $\omega_{\vec{k}j}$ is the frequency of the normal mode. For LO phonon modes, the decay occurs mainly through the creation of two longitudinal-acoustic (LA) modes. At the same time, the normal process dominates over the umklapp process when the LO phonon wavevector is small. Retaining only this term, the decay Hamiltonian for LO phonons becomes

$$H_{\vec{k},\vec{k}',\vec{k}''} = \frac{1}{\sqrt{N}} \left[\frac{\hbar}{2m}\right]^{3/2} \left[\frac{1}{\omega_{\vec{k}}\omega_{\vec{k}'}\omega_{\vec{k}''}}\right]^{1/2} P(\vec{k},\vec{k}',\vec{k}'')\, a_{\vec{k}} a^{\dagger}_{\vec{k}'} a^{\dagger}_{\vec{k}''}\, e^{i(\vec{k}-\vec{k}'-\vec{k}'')\cdot\vec{r}} . \tag{10}$$

The indices for mode polarization have been removed since only one decay path has been considered (i.e., $\vec{k}_{LO} \rightarrow \vec{k}'_{LA} + \vec{k}''_{LA}$). Contributions by other processes can be formulated easily from Eq. (8).

In the interaction Hamiltonian derived above, all the terms other than $P(\vec{k};\vec{k}';\vec{k}'')$ are known. However, it is quite difficult, if not impossible, to properly measure the anharmonic potential term. To circumvent this problem, Keating [13] has used the theory of elasticity since there exists a relationship between the third order elasticity coefficients and the anharmonic term in the crystal potential. Elasticity coefficients also are related closely to the Grüneisen parameter. From the analysis, the strain energy density U_a associated with the third order contributions in cubic crystals reduces to [13]

$$U_a = \frac{1}{6}C_{111}(e_1^3 + e_2^3 + e_3^3) + \frac{1}{2}C_{112}[e_1^2(e_2 + e_3) + e_2^2(e_3 + e_1) + e_3^2(e_1 + e_2)] + C_{123}e_1e_2e_3 \tag{11}$$

$$+ \frac{1}{2}C_{144}(e_1e_4^2 + e_2e_5^2 + e_3e_6^2) + \frac{1}{2}C_{166}[e_1(e_5^2 + e_6^2) + e_2(e_6^2 + e_4^2) + e_3(e_4^2 + e_5^2)]$$

$$+ C_{456}e_4e_5e_6 + \frac{1}{2}C_{11}(e_1^3 + e_2^3 + e_3^3) + \frac{1}{2}C_{12}[e_1^2(e_2 + e_3) + e_2^2(e_3 + e_1) + e_3^2(e_1 + e_2)] ,$$

where C_{JKL} (C_{JK}) are the third (second) order elastic constants, respectively, and e_J represents the linear part of the strain variable as defined in Ref. 13. A careful comparison of Keating's formulation with that of a microscopic model by Tua and Mahan [11] reveals that U_a corresponds to P as defined in Eq. (8); accordingly, a valid expression for the decay Hamiltonian can be developed once U_a is evaluated. In general, the values for the second order and third order elastic constants can be obtained from the literature. At the same time, the magnitude of the strain variable e_J may be estimated based on numerical models for lattice dynamics such as the valence shell model. Based on the Hamiltonian derived above, the LO phonon decay rate can be calculated readily by following Fermi's golden rule approximation. Then, the lifetime for the LO phonon with wavevector $\vec{k}$ may be defined as

$$\frac{1}{\tau_p} = \sum \frac{\pi\hbar^2 U_a^2}{4Nm^3} \left[\frac{1}{\omega_{\vec{k}}\omega_{\vec{k}'}\omega_{\vec{k}''}} \right] (1 + n_{\vec{k}'} + n_{\vec{k}''}) \, \delta_{\vec{k},\vec{k}'+\vec{k}''} \, \delta(\hbar\omega_{\vec{k}} - \hbar\omega_{\vec{k}'} - \hbar\omega_{\vec{k}''}) , \qquad (12)$$

where $n_{\vec{k}'}$ is the normal Bose-Einstein phonon occupation number. When more than one path exists for decay (i.e., paths other than LO→LA+LA), each contribution is added to obtain the LO phonon lifetime. In this case, the sum in Eq. (12) is over both the phonon wavevector and mode polarization.

Using this formalism, we have calculated the lifetimes of bulk LO phonons in GaAs. In these calculations, the values for e_J have been estimated based on our previous work on the valence shell model (which was discussed in detail in our report last year). Although elastic constants for GaAs are available in the literature, some of the measured third-order constants (C_{123} and C_{144} in particular) show wide variations. To circumvent this uncertainty, we have used a relationship between the third order elastic constants and the microscopic force constants developed by Keating [13], and have chosen an optimum set systematically. The values adopted in this study are listed in Table I. These values

Table I. Third-order elastic constants for GaAs in the unit of GPa.

C_{111}	C_{112}	C_{123}	C_{144}	C_{155}
-663	-391	-11	-41	-311

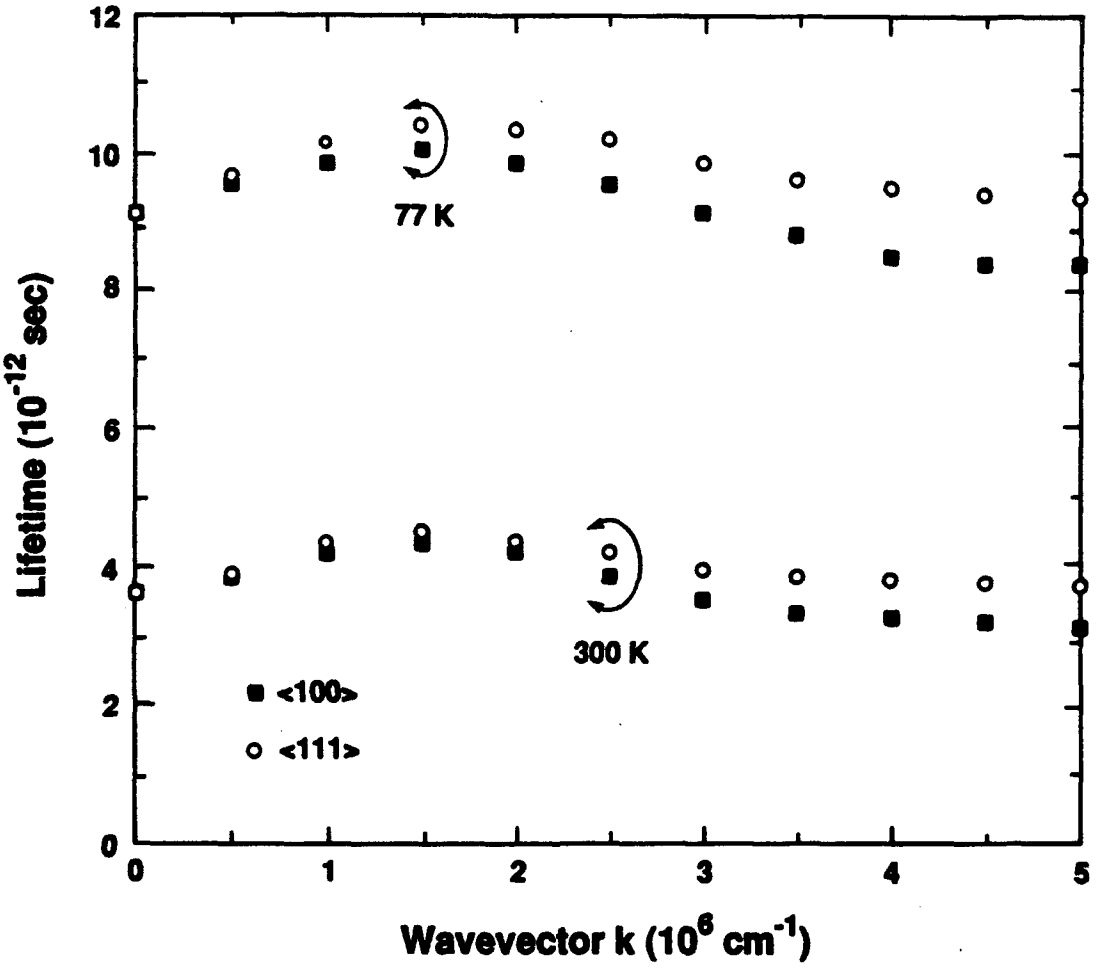

Figure 3. LO phonon lifetime as a function of wavevector in bulk GaAs along the <100> and <111> directions at 77 K and 300 K.

are well within the range of experimental variations. Figure 3 shows the LO phonon lifetime as a function of wavevector in bulk GaAs along the <100> and <111> directions at 77 K and 300 K. Since the decay into two LA phonons is the dominant process, we have considered only this mechanism. The other processes are either not possible (when energy and momentum cannot be conserved) or provide a small contribution to the overall lifetime. As can be seen, the lifetime decreases with increasing temperature mainly due to the Bose-Einstein occupation number. The results obtained from our analysis agree well with the widely accepted experimental data (3.5 ps at 300 K and 7 ps at 77 K). The agreement is better at room temperature than at low temperatures. This is reasonable since the third-order elastic constants used in our study are estimated at 300 K. Although elastic constants depend on temperature, their values are not provided over a wide range of temperature. Thus, it is likely that if temperature-dependent elastic constants become available, the accuracy of calculation can be enhanced particularly at low temperatures. At the same time, inclusion of other decay mechanisms (i.e., other than an LO phonon decaying into two LA phonons) reduces the lifetime by approximately 0.5 ps and, thus, further improves the agreement. From the figure, it is also found that the phonon lifetime does not depend strongly on the phonon wavevector. As a result, the k=0 value provides a good approximation for the LO phonon lifetime in bulk materials.

Phonon-assisted Γ-X transition rates in type-II superlattices

The relaxation rates of photoexcited electrons is an important issue because of its fundamental nature as well as for possible device applications. Contrary to the case of type-I heterostructures, the electrons in type-II structures are excited to a direct-gap energy level (Γ) in one layer and then can relax to an indirect-gap energy level (X) in the adjacent layer. This case is potentially significant for device applications since electron relaxation occurs in conjunction with real-space transfer. This process, which is normally forbidden, is now possible due to the mixing of Γ and X states by the superlattice potential and relaxation of momentum conservation due to interface disorder (lateral mixing).

Several experimental results related to Γ-X transfer are available in the literature. In spite of the spatial charge transfer, the relaxation rate can be very high. To this date, there has been relatively little theoretical effort to analyze the Γ-X transfer in type-II structures. Recently, we have calculated the Γ-X scattering rates due to optical phonon emission using a realistic band structure model (tight binding), and have demonstrated that this is an important mechanism for the Γ-X relaxation process in type-II superlattices.

The electron-phonon interaction in low-dimensional systems is altered strongly due to the confinement of the carriers and the confinement of the phonons. Usually, a single-band, spherical effective-mass model is used for the description of the confined carrier states. It is commonly assumed that each of these states is derived from bulk states of a given symmetry only (e.g., Γ, X, or L), and levels derived from different bulk states do not interact with each other. In a superlattice, momentum in the growth direction is not conserved due to the discontinuities in the superlattice potential in this direction. Therefore, bulk states of the same energy but different symmetry can couple with each other. As a result, the envelope-function approximation, which works very well in many cases, is not suitable in this case. In our study, a second nearest neighbor empirical tight binding method with an sp^3 basis was used for describing the electronic band structure [14]. The mixing of the Γ and X valleys is intrinsically included in this model since the complete band-structure is described in the tight binding method. For a proper calculation of the electron-phonon scattering rates, the effects of phonon confinement should also be taken into account. Although we have developed a microscopic model for lattice dynamics, using this model in the calculation of electron-phonon interactions coupled with a realistic electronic band structure requires intensive computation. Therefore, for the description of phonon confinement, we used the dielectric continuum (slab) model because of its simplicity and reasonable accuracy. In the dielectric continuum model picture, the confined modes are totally confined within an individual layer, and the phonon potential of one type of layer is identically zero in the adjacent layer. Hence, phonon potentials in each well do not interact with each other, and consequently,

confined phonon modes in a superlattice are the same as the ones for a quantum well in this picture. The interface phonon modes in a superlattice, on the other hand, are modified due to the periodicity of the structure and the overlapping of potentials [15]. In this case, the phonon potential extends over the whole superlattice. The resulting Hamiltonian due to interacting interface modes is very complicated. To simplify the calculations, we considered only the case where the phonon wavevector along the growth direction (i.e., the wavevector in the superlattice miniband) is zero. Based on this interaction Hamiltonian, we calculated the electron scattering rate due to optical phonon emission following Fermi's Golden Rule. To perform the summation, we made use of the fact that the phonon potentials vary slowly in the unit cell compared with the atomic orbitals which are strongly localized at atomic locations. The sum over all possible finite states within the 2-D Brillouin zone was evaluated numerically [16].

The specific structure of interest in our initial calculations was a superlattice with M monolayers of GaAs and N monolayers of AlAs. The energy levels at the miniband minimum obtained from the tight binding calculation as a function of AlAs layer thickness are shown in Fig. 4. The GaAs layer thickness was kept constant at 8 monolayers. The levels are labeled as Γ and X following the effective mass notation, although each level is actually a combination of these two bulk states. Here, the superlattice states are labeled after the dominant of the two bulk states forming them. As can be seen, the effect of changing the AlAs layer thickness is to make the energy difference, hence, the interaction between the lowest Γ level (Γ_1) and the X levels vary. The parity behavior of states needs to be mentioned briefly because of the effect of parity on the overlap of electronic wave functions. In the superlattice, the electronic wave functions have definite parity only when the electron is at the miniband minimum or miniband maximum. When the initial state for the electron is assumed to be the bottom of the miniband, the parity of the Γ_1 state is even, regardless of AlAs layer thickness. The parity of the X levels, on the other hand, depends on the number of AlAs monolayers. The X_i levels with odd

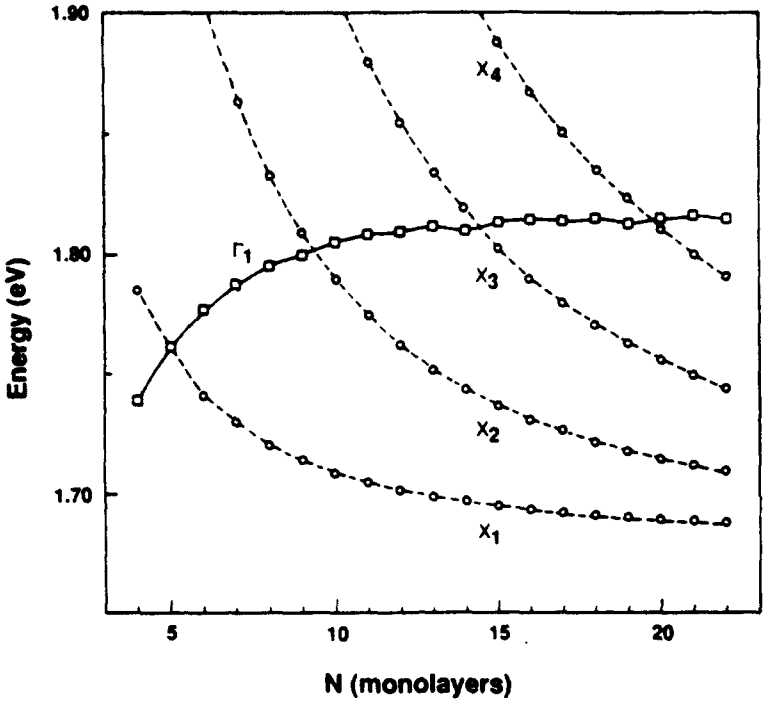

Figure 4. Energy levels obtained from the tight binding calculation as a function of AlAs layer thickness. The GaAs thickness is fixed at 8 monolayers. The discrete energy levels are marked as Γ and X after the more dominant one of the two bulk states making up the confined state.

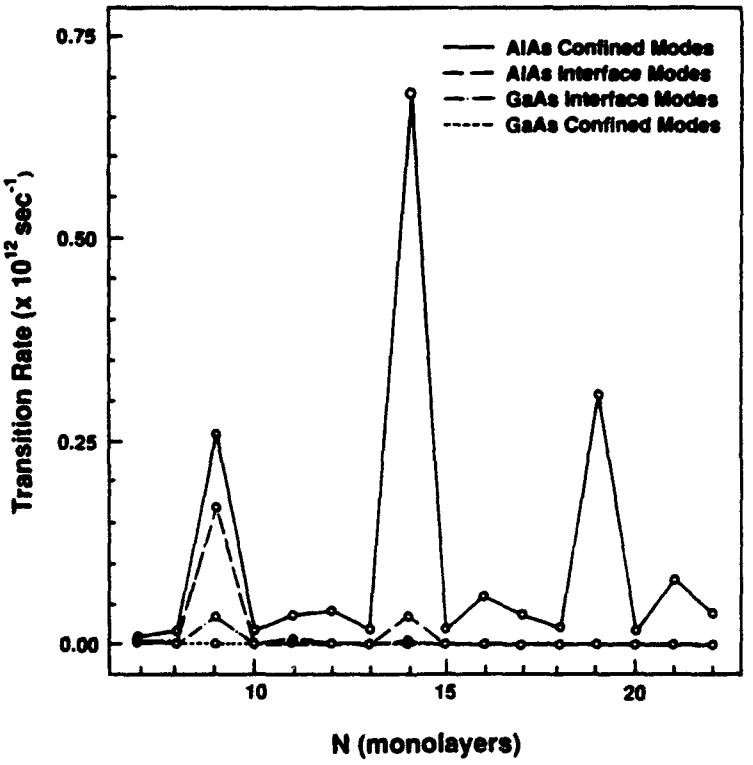

Figure 5. Γ_1–X_1 transition rate due to optical phonon emission as a function of AlAs layer thickness. The GaAs thickness is 8 monolayers throughout.

(even) i have the same (opposite) parity as N. The parity behavior of states is important because the states of opposite parity do not mix strongly.

Scattering rates due to the emission of different phonon modes are shown in Fig. 5. The results presented are the sums of contributions by all normal modes for a given type of phonon. In calculating the intersubband scattering rates, the electron is taken to be initially at the bottom of the Γ_1 subband. It then transfers to the X_1 subband by emitting an optical phonon. As is apparent from Figs. 4 and 5, the scattering rate is strongest when the Γ and X levels are closest in energy. Under this condition, the levels interact very strongly with each other and the Γ level has large X character. Therefore, the overlap between the initial and final states is large. This interaction and the resulting large overlap decreases rapidly as the energy separation increases. This is one of the two reasons for strong thickness dependence (the other being parity) of the scattering rate. Among different phonon modes, the AlAs confined modes are strongest, followed by the AlAs interface modes. The GaAs modes are weaker, with the GaAs confined modes being the weakest. This is due to the fact that the final state X_1 wave function is strongly confined within the AlAs layers. Consequently, the overlap involving GaAs confined modes is very small. An interesting point to note about Fig. 5 is that the dominant phonon modes alternate between being even and odd. This is because the parity of the X level alternates as the AlAs thickness is changed by one monolayer each time. For even (odd) AlAs layer thickness, the parity of the lowest X level is even (odd); hence, the even (odd) phonon modes are strong. The effect of parity can be also be observed at cross-over points where the Γ and X level energies become very close. From Fig. 4, it is seen that the two levels have almost the same energy for N=5, but they do not mix and repel each other. This is because Γ_1 and X_1 have the opposite parities for this thickness. For other thicknesses where the two levels become close, however, they do repel each other because they have the same parity. This is the reason why the scattering rate for N=19 is much stronger than for N=20. Finally, we compared our results with an experiment by de Paula [17] where

the Γ to X transition rate via phonon emission was obtained by a time-resolved anti-Stokes measurement. For the case of M=8 and N=14, they found the transfer time to be around 1 ps, which is in agreement with the rate calculated in this study.

Extension of Kronig-Penny model for Γ-X mixing in type-II superlattices

As discussed in the previous section, an accurate description of band structure including Γ-X mixing is essential for the investigation of electronic and optoelectronic properties in type-II superlattices. For the conduction bands of superlattices made of direct-gap materials (i.e., type-I), the Kronig-Penney has been used satisfactorily to understand many important problems. However, other complicated methods (such as the empirical tight binding method used in the previous section) are required to model the superlattice when this is not the case. An accurate yet simple model for treating mixing effects is useful to make theoretical predictions and explain the experimental results. Therefore, it is very desirable to extend the Kronig-Penney model so that mixings of different valleys may be treated. We developed such an extension in which the energy bands and wave functions in type-II superlattices are calculated adopting a simplified approach formulated by Cho and Prucnal [18] along with the boundary conditions introduced by Liu [19] in treating single barrier tunneling. Our model has the merit of being easy to implement and permits the wave functions to be expressed analytically. Therefore, it can be a valuable tool for simple and efficient calculations of mixing effects.

In a superlattice, the electronic state is frequently approximated by a mixture of the related zone-center (Γ) and zone-edge (X) bulk states. Accordingly, the wave function, ψ, is written as the sum of the products of slowly varying envelope functions and band edge periodic functions (Bloch functions): i.e., $\psi = \psi_\Gamma u_\Gamma + \psi_X u_X$, where u_Γ and u_X are the Bloch functions for the Γ and X valleys, respectively. In vector notation, the wave function may be expressed as $\psi = (\psi_\Gamma, \psi_X)$. The coupling of Γ and X valleys due to the broken translational symmetry of the crystal can be modeled by the off-diagonal elements in the potential energy [19]. For simplicity, these off-diagonal terms are represented by delta

functions centered at the interfaces:

$$V = \begin{bmatrix} V_\Gamma(z) & \alpha\delta(z) \\ \alpha\delta(z) & V_X(z) \end{bmatrix}, \tag{13}$$

where z is the direction of crystal growth, α is a parameter quantifying mixing, $\delta(z)$ is the Dirac delta function, and $V_\Gamma(z)$ and $V_X(z)$ define the Γ-potential discontinuity and X-potential discontinuity, respectively. The wave (envelope) function continuity condition (at z=0) is,

$$\begin{bmatrix} \psi_\Gamma \\ \psi_X \end{bmatrix}_{0-} = \begin{bmatrix} \psi_\Gamma \\ \psi_X \end{bmatrix}_{0+}. \tag{14}$$

The other boundary condition can be derived by integration of the Schrödinger equation across the interface:

$$-\frac{\hbar^2}{2}\left[\frac{1}{m_\Gamma(z)}\frac{\partial\psi_\Gamma}{\partial z}\Big|_{0+} - \frac{1}{m_\Gamma(z)}\frac{\partial\psi_\Gamma}{\partial z}\Big|_{0-}\right] + \alpha\psi_X = 0, \tag{15}$$

$$-\frac{\hbar^2}{2}\left[\frac{1}{m_X(z)}\frac{\partial\psi_X}{\partial z}\Big|_{0+} - \frac{1}{m_X(z)}\frac{\partial\psi_X}{\partial z}\Big|_{0-}\right] + \alpha\psi_\Gamma = 0.$$

As can be seen, introduction of the delta function potential results in a boundary condition in which the Γ and X valleys are coupled across the interface. In obtaining this result, it is assumed that the Bloch functions of the respective band edges in the two constituent materials do not differ significantly.

With our model, we obtained analytical expressions for the envelop functions and a transcendental equation for the energy levels. The energies of the lowest Γ and X levels are shown in Fig. 6 as a function of layer thickness with and without mixing. In this figure, α equals 0.1 eV-Å; as discussed below, this is a reasonable value in light of the favorable agreement with numerous experimental and theoretical results. As can be noticed, the effect of mixing is to create an anticrossing behavior where the two levels are expected to meet. This important feature is correctly reflected in our treatment. We also demonstrated that the wave functions in type-II superlattices obtained from conventional Kronig-

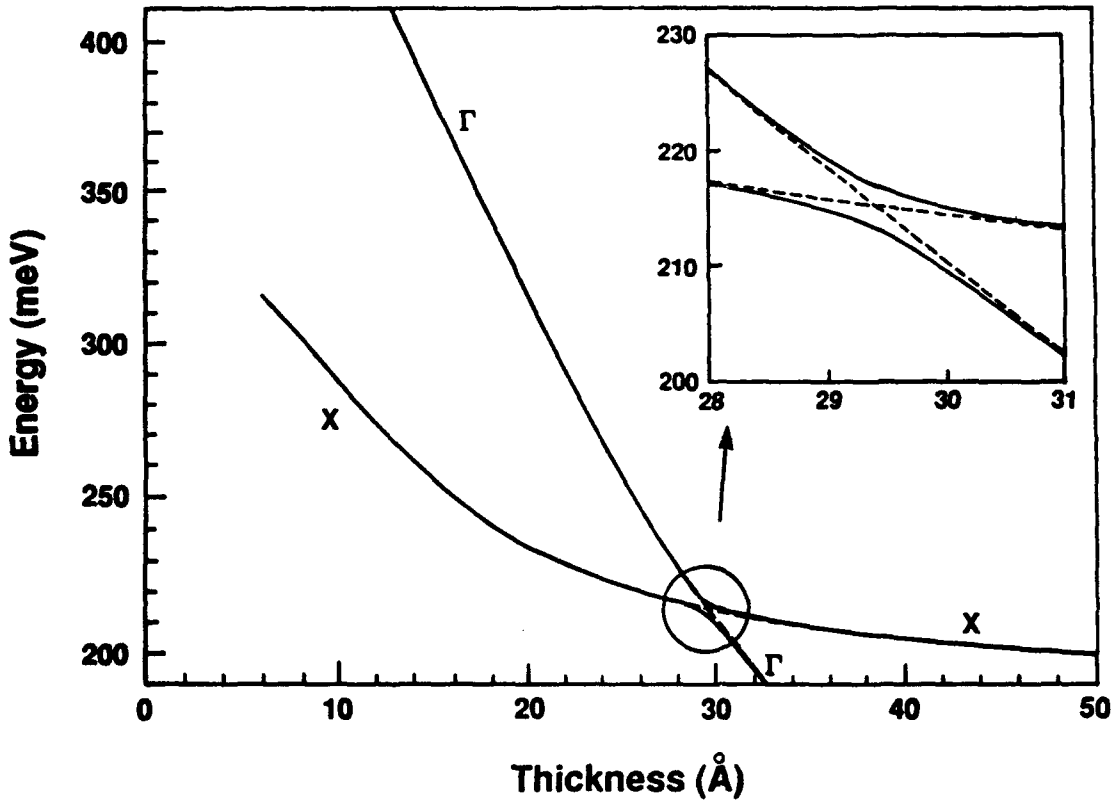

Figure 6. Energies at the miniband minimum for the two lowest levels in a GaAs/AlAs superlattice as a function of layer thickness. The GaAs and AlAs layers are assumed to be of equal thickness. Higher energy levels are omitted in this figure for clarity. Solid lines show the bands with α=0.1 eV-Å, while the energies for dashed lines are obtained by setting α equal to 0 (i.e., conventional Kronig-Penney model). The inset shows the anticrossing behavior in detail and has the same labels and the units as the main figure.

Penney model are considerably in error when the layer thicknesses are such that strong mixing of Γ and X states occurs. Near the point of anticrossing, it is imperative that the interaction of the two valleys be considered to have correct wave functions. Our model, as opposed to the conventional Kronig-Penney model, yields appropriate wave functions for the mixed states. We obtained the value of our mixing parameter (the only adjustable parameter in our model) by comparison with both experiments and more sophisticated theoretical models. The values of α deduced from a variety of sources converged around a single value (0.1 eV-Å) of this parameter. As a result, we showed that the simple and efficient model we developed could reasonably reproduce the important aspects of valley mixing effects in type-II superlattices.

Theory of Bloch electron dynamics in electric fields

Bloch electron dynamics in electric fileds has been a subject of great interest dating back to the earliest applications of quantum mechanics to solid state physics [1]. Even more recently, as modern fabrication technologies continue to drive the study of solid state transport into the nanometer domain, many new and interesting questions have emerged concerning the solid state dynamics and quantum transport of carriers in band-engineered superlattices and tailored periodic solids.

In the past year, we have developed a novel formalism for treating Bloch electron dynamics and quantum transport in a superimposed uniform and oscillatory electric field $\vec{E}(t) = \vec{E}_o + \vec{E}_1 \cos\omega t$. In the formalism, the electric field is described through the use of the vector potential, and a basis set of localized, electric field-dependent Wannier, and related envelope function is developed and utilized to describe the dynamics. From the theory, a complete analysis of single-band and multi-band processes is derived for a Bloch electron in the presence of a superimposed uniform and oscillatory electric field. In the single-band approximation, it is shown that the tuning of the oscillatory field frequency ω to some multiple N_o of the Bloch frequency $\omega_B = eE_oa/\hbar$ results in the resonant displacement of the electron from a given site l_o to the tuned multiple of lattice sites $l_o \pm N_o a$ along with a concomitant

development of a DC velocity in the direction of the electric field for the initial Bloch state,

$$\langle \vec{v}_n \rangle_x^{DC} = \frac{2a}{\hbar} \sum_{m>0} c_n(mN_o a, \vec{K}_{o\perp})\, (mM)\, (-1)^m\, J_m(mN_o\alpha)\, \sin(mN_o K_{ox} a)\,, \tag{16}$$

where J_m is the Bessel function of integer order m, $\alpha = eE_1 a/\hbar\omega$, and the energy band function and its Fourier components are defined as

$$\varepsilon_n(\vec{K}) = \varepsilon_n(K_x, \vec{K}_\perp) = \sum_{l_x} c_n(l_x, \vec{K}_\perp)\, e^{iK_x l_x} = \sum_{l_x} e^{iK_x l_x} \sum_{\vec{l}_\perp} c_n'(\vec{l})\, e^{i\vec{K}_\perp \cdot \vec{l}_\perp}\,. \tag{17}$$

On the other hand, for a fixed oscillatory field frequency ω, the DC current can occur in the direction of the electric field by tuning the Bloch frequency ω_B (DC field strength E_o) to some multiple of the oscillatory field frequency (i.e., $\omega_B = M_o\omega$). The DC velocity for initial Bloch state is found to be

$$\langle \vec{v}_n \rangle_x^{DC} = -\frac{2a}{\hbar} \sum_{l_x>0} (-1)^{M_o l_x}\, c_n(l_x, \vec{K}_{o\perp})\, J_{l_x M_o}(l_x\alpha)\, l_x\, \sin(l_x K_{ox} a)\,. \tag{18}$$

For the one-dimensional nearest-neighbor tight-binding model, the DC velocity is

$$\langle \vec{v}_n \rangle^{DC} = -\frac{2a c_n'(a)}{\hbar}\, J_o(\alpha)\, \sin(K_o a)\,, \tag{19}$$

which resembles the usual Bloch velocity with a deformed band parameter $\tilde{c}_n'(a) = c_n'(a) J_o(\alpha)$.

Further, from the multi-band analysis, a generalized transition rate is derived in terms of the DC field, oscillatory field, and the relevant band parameters, showing all possible transitions include Zener tunneling, photon assisted tunneling, multiphoton emission/absorption, as well as transitions between states of the Wannier ladder. Based on the methodology which was developed and presented in our earlier report, the multi-band coupling is treated in the Wigner-Weisskopf approximation, which allows for the analysis of the long-time, time-dependent tunneling characteristics of an electron transition out of an initially occupied band due to power absorbed by the electric field, while preserving conservation of total transition probability over the complete set of excited bands. The total transition rate for an electron to tunnel out of the initially occupied band is derived, and the results show the dependence of

the transition rate on the initial condition of the system and the decay rate of the initial band amplitude, $\gamma_n(\vec{K})$, which is given as,

$$\gamma_n(\vec{K}) = 2\pi \sum_{n' \neq n} \left\{ |D_{nn'}(0,\vec{K}_\perp)|^2 \left(\frac{eE_o}{\hbar}\right)^2 \delta[\tilde{\omega}_{nn'}(\vec{K})] \right. \tag{20}$$

$$+ \frac{1}{4} |D_{nn'}(0,\vec{K}_\perp)|^2 \left(\frac{eE_1}{\hbar}\right)^2 [\delta(\tilde{\omega}_{nn'}(\vec{K})+\omega) + \delta(\tilde{\omega}_{nn'}(\vec{K})-\omega)]$$

$$\left. + \sum_{l_x \neq 0} \sum_m |D_{nn'}(l_x,\vec{K}_\perp)|^2 J_m^2(l_x\alpha) \left(\frac{eE_o}{\hbar} + \frac{eE_1}{\hbar}\frac{m}{l_x\alpha}\right)^2 \delta[\tilde{\omega}_{nn'}(\vec{K}) - l_x\omega_B - m\omega] \right\}.$$

It is noted that $\gamma_n(\vec{K})$ consists of several δ functions, which indicate the possible physical processes for a Bloch electron in a homogeneous, time-varying electric field. The first term in $\gamma_n(\vec{K})$ indicates the interband transition due to Zener tunneling between the deformed bands n and n′, which is proportional to E_o^2. Here, $D_{nn'}(l_x,\vec{K}_\perp) = \frac{i}{4} a e^{-qa|l_x|}$, $\varepsilon_n(q,\vec{K}_\perp) = \varepsilon_{n'}(q,\vec{K}_\perp)$, and $\tilde{\omega}_{nn'} = [\tilde{\varepsilon}_{n'}(\vec{K}) - \tilde{\varepsilon}_n(\vec{K})]/\hbar$ with the deformed energy band function,

$$\tilde{\varepsilon}_n(\vec{K}) = \sum_{l_x} \sum_m c_n(l_x,\vec{K}_\perp)\, J_m(l_x\alpha)\, e^{i l_x K_x a}, \tag{21}$$

where $l_x\omega_B + m\omega = 0$. The second and third terms in $\gamma_n(\vec{K})$ indicate the transitions between the two deformed bands through absorption/emission of a photon, which are proportional to E_1^2, and the last term suggests the interband transitions between the deformed bands via Wannier-Stark transitions, as well as multiphonon absorption/emission. The Franz-Keldysh effect can also be explained from the results.

In addition to Bloch electron dynamics in a homogeneous, time varying electric field, we have investigated the effect of localized impurities on the transport of an electron in a uniform electric field $\vec{E}_o$. We have developed a theory to describe Bloch electron transport through spatially localized inhomogeneous potential barriers. In applying the theory, field-dependent envelope functions and currents for a Bloch electron tunneling through single and double Slater-Koster potential barriers are derived

using the Wannier representation within the one-dimensional nearest-neighbor tight-binding approximation. The exact solutions for the envelope functions in the Wannier representation are expressed in an integral form through the use of the Laplace transform solutions for the envelope functions at the impurity sites. Early time solutions are obtained for the envelope functions and the velocity is calculated for the given fields. The asymptotical behaviors for high-field and low-field limits are observed.

To study the effects of the localized potential barriers on the Wannier-Stark levels, we have derived the electric field dependent Green's function for the one-dimensional nearest-neighbor tight-binding band, $\varepsilon(\vec{K}) = \varepsilon_o + 2\varepsilon_1 \cos Ka$, which is

$$W_n^+(l,l') = \frac{\pi(-1)^{l'}}{\hbar\omega_B} J_{-l'-y}\left(\frac{2\varepsilon_1}{\hbar\omega_B}\right) J_{l'+y}\left(\frac{2\varepsilon_1}{\hbar\omega_B}\right) \left\{P\left(\frac{1}{\sin\pi y}\right) - i\sum_m \delta(y-m)\right\}, \qquad (22)$$

where $y = (E-\varepsilon_o)/\hbar\omega_B$. The Stark energy spectra for single and double Slater-Koster impurities are calculated using the field-dependent Green's function. The results show that for relatively low potential barriers and high electric field, the energy levels are almost uniform, resembling the Wannier-Stark ladder, and the barriers act as perturbations; for relatively low field and high potential barriers, the Wannier-Stark uniformity of the levels becomes distorted (see Fig. 7). Although the illustrations cited here are for Slater-Koster barriers, the calculation is easily extended to general, localized potentials.

2.3 Publications and Presentations

During the last year, this program has resulted in nine refereed publications in the literature, five additional manuscripts are currently in press, and one more has been submitted to a major technical journal. Ten presentations and invited talks have been given at conferences and workshops. The following paragraphs summarize the publications and presentations made under this program during the past contract period.

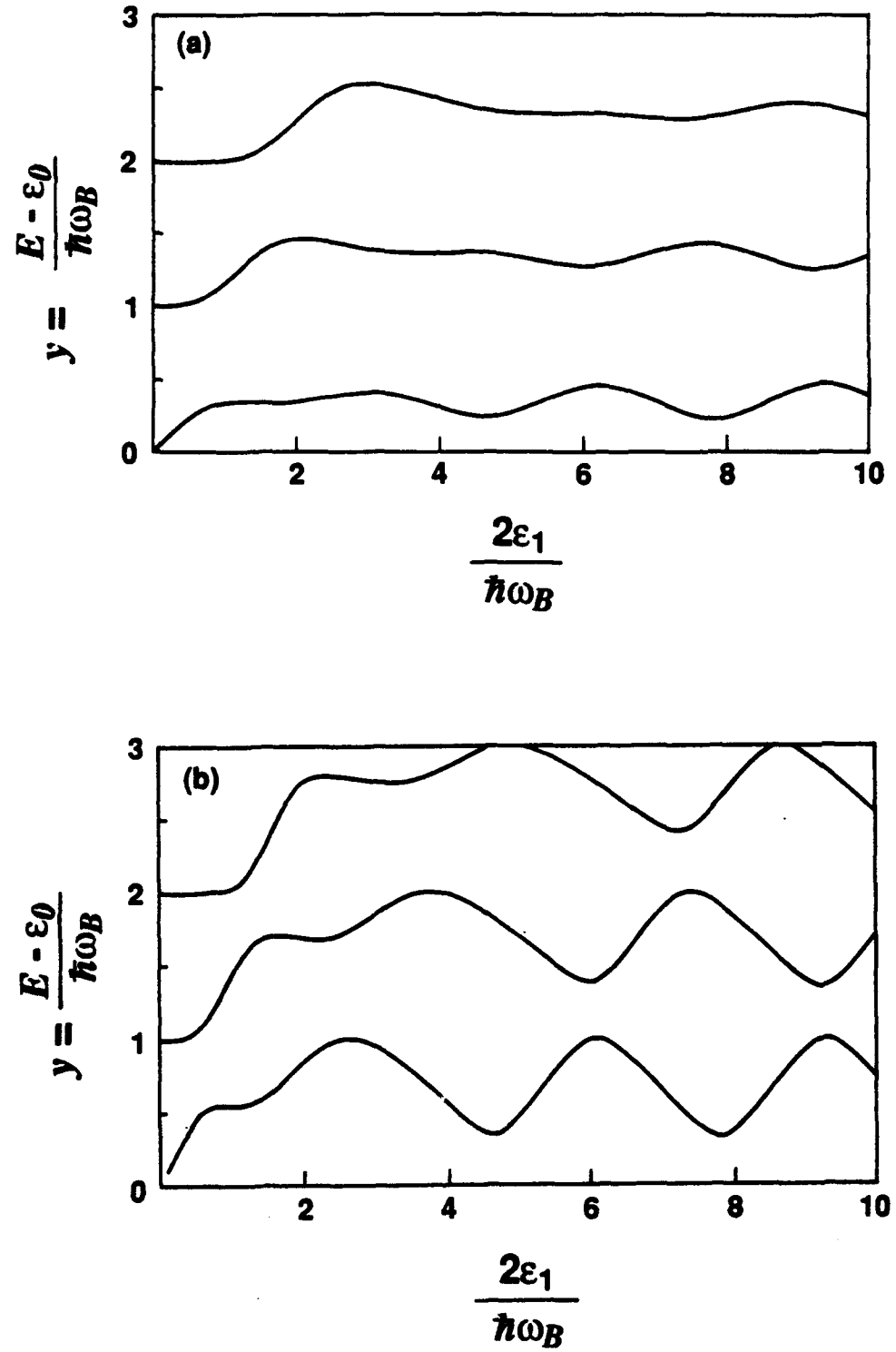

Figure 7. Wannier-Stark energy levels for two impurities of two lattice spacing apart with the relative impurity strength of (a) $V_o/2\varepsilon_1 = 0.5$ and (b) $V_o/2\varepsilon_1 = 1.0$.

A. Refereed Publications

M. U. Erdogan, K. W. Kim, M. A. Stroscio, and M. Dutta, "An Extension of Kronig-Penney Model for Γ-X Mixing in Superlattices," *J. Appl. Phys.* 74, 4777 (1993).

A. R. Bhatt, K. W. Kim, M. A. Stroscio, and J. M. Higman, "Simplified Microscopic Model for Electron-Optical-Phonon Interactions in Quantum Wells," *Phys. Rev. B* 48, 14671 (1993).

M. A. Stroscio, G. J. Iafrate, K. W. Kim, S. Yu, V. Mitin, and N. Bannov, "Scattering of Carriers from Confined Acoustic Modes in Nanostructures," in *Proceedings of the 1993 Intl. Semiconductor Device Research Symp.*, edited by M. Shur and E. Towe (Univ. of Virginia, Charlottesville, Virginia, 1993), pp. 873-875.

M. A. Stroscio and K. W. Kim, "Generalized Piezoelectric Scattering Rate for Electrons in a Two-Dimensional Electron Gas," *Solid-State Electron.* 37, 181 (1994).

J. He, G. J. Iafrate, and M. A. Littlejohn, "Multi-Band Theory of Bloch Electron Dynamics in Electric Fields," *Semicond. Sci. Technol.* 9, 815 (1994).

M. U. Erdogan, V. Sankaran, K. W. Kim, M. A. Stroscio, and G. J. Iafrate, "Real-Space Transfer of Photoexited Electrons in Type-II Superlattices via Optical-Phonon Emission," *Proc. SPIE* 2146, 34 (1994).

K. W. Kim, S. Yu, M. U. Erdogan, M. A. Stroscio, and G. J. Iafrate, "Acoustic Phonons in Rectangular Quantum Wires: Approximate Compressional Modes and the Corresponding Deformational Potential Interactions," *Proc. SPIE* 2142, 77 (1994).

M. U. Erdogan, V. Sankaran, K. W. Kim, M. A. Stroscio, and G. J. Iafrate "Phonon-Assisted Γ-X Transition Rates in Type-II Superlattices," *Phys. Rev. B* 50, 2485 (1994).

S. Yu, K. W. Kim, M. A. Stroscio, G. J. Iafrate, and A. Ballato, "Electron-Acoustic-Phonon Scattering Rates in Rectangular Quantum Wires," *Phys. Rev. B* 50, 1733 (1994).

M. A. Stroscio, K. W. Kim, S. Yu, and A. Ballato, "Quantized Acoustic Phonon Modes in Quantum Wires and Quantum Dots," accepted for publication in *J. Appl. Phys.*

A. R. Bhatt, K. W. Kim, and M. A. Stroscio, "Theoretical Calculation of Longitudinal-Optical Phonon Lifetime in GaAs," accepted for publication in *J. Appl. Phys.*

J. He and G. J. Iafrate, "Multi-Band Theory of Bloch Electron Dynamics in a Homogeneous Electric Field," accepted for publication in *Phys. Rev. B.*

V. Sankaran, K. W. Kim, and G. J. Iafrate, "Tight-Binding Calculation of Linear Optical Properties of $In_xGa_{1-x}As$ Alloys and Heterostructures," to be published in *Proceedings of the 21th Intl. Symp. on Compound Semiconductors.*

J. He and G. J. Iafrate, "Effects of Band-Structure and Electric Fields on Resonant Tunneling Dynamics," to be published in *NATO ASI Series Volume: Quantum Transport in Ultrasmall Devices.*

M. U. Erdogan, K. W. Kim, and M. A. Stroscio, "Strain Effects on Hole Tunneling Dynamics in Double Barrier Heterostructures," submitted to *J. Appl. Phys.*

B. Conference Presentations

M. A. Stroscio, G. J. Iafrate, K. W. Kim, S. Yu, V. Mitin, and N. Bannov, "Scattering of Carriers from Confined Acoustic Modes in Nanostructures," presented at the 1993 Intl. Semiconductor Device Research Symp. (December, 1993, Charlottesville, Virginia).

M. U. Erdogan, V. Sankaran, K. W. Kim, M. A. Stroscio, and G. J. Iafrate, "Real-Space Transfer of Photoexited Electrons in Type-II Superlattices via Optical-Phonon Emission," presented at the SPIE OE/LASE '94: Physics and Simulation of Optoelectronic Devices II (January, 1994, Los Angeles, Calif.).

K. W. Kim, S. Yu, M. U. Erdogan, M. A. Stroscio, and G. J. Iafrate, "Acoustic Phonons in Rectangular Quantum Wires: Approximate Compressional Modes and the Corresponding Deformational Potential Interactions," presented at the SPIE OE/LASE '94: Ultrafast Phenomena in Semiconductors (January, 1994, Los Angeles, Calif.).

M. A. Stroscio, G. J. Iafrate, K. W. Kim, S. Yu, A. Ballato, M. Dutta, V. Mitin, and N. Bannov, "Acoustic Phonons in Mesoscopic Structures," presented at the March Meeting of the American Physical Society (March, 1994, Pittsburgh, Penn.).

A. R. Bhatt, K. W. Kim, and M. A. Stroscio, "Theoretical Calculation of Lifetimes for GaAs and GaP," presented at the March Meeting of the American Physical Society (March, 1994, Pittsburgh, Penn.).

J. He and G. J. Iafrate, "Bloch Electron Dynamics in a Superimposed Uniform and Oscillatory Electric Field," presented at the March Meeting of the American Physical Society (March, 1994, Pittsburgh, Penn.).

G. J. Iafrate and J. He, "Effects of Electric Fields on Resonant Tunneling," presented at the March Meeting of the American Physical Society (March, 1994, Pittsburgh, Penn.).

M. A. Stroscio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, and H. L. Grubin, "Confined and Interface Phonons and Their Interactions with Carriers as Modified by Surfaces and Interfaces in Mesoscopic Structures (Invited)," presented at the Conference on Surfaces and Interfaces in Mesoscopic Devices (April, 1994, Kona, Hawaii).

M. A. Stroscio, G. J. Iafrate, K. W. Kim, S. Yu, V. Mitin, and N. Bannov, "Scattering of Carriers from Confined Acoustic Modes in Nanostructures (Invited)," presented at the 2nd Intl. Symp. on Quantum Confinement: Physics and Applications (May, 1994, San Francisco, Calif.).

J. He and G. J. Iafrate, ""Effects of Band-Structure and Electric Fields on Resonant Tunneling Dynamics (Invited)," presented at the NATO ASI on Quantum Transport in Ultrasubmicron Devices (July, 1994, Il Ciocco, Italy).

V. Sankaran, K. W. Kim, and G. J. Iafrate, "Tight-Binding Calculation of Linear Optical Properties of

$In_xGa_{1-x}As$ Alloys and Heterostructures," to be presented at the 21st Intl. Symp. on Compound Semiconductors (September, 1994, San Diego, Calif.).

2.4 List of References

[1] J. B. Krieger and G. J. Iafrate, Phys. Rev. B33, 5494 (1986); Phys. Rev. B35, 9644 (1987); G. J. Iafrate and J. B. Krieger, Solid-State Electron. 31, 517 (1988); Phys. Rev. B40, 6144 (1989).

[2] L. F. Register, M. A. Littlejohn, and M. A. Stroscio, Superlatt. Microstruct. 4, 61 (1988).

[3] B. A. Mason and K. Hess, Phys. Rev. B39, 5051 (1989).

[4] J. Seyler and M. N. Wybourne, Phys. Rev. Lett. 69, 1427 (1992); Z. V. Popvic, J. Spitzer, T. Ruf, M. Cardona, R. Notzel, and K. Ploog, Phys. Rev. B48, 1659 (1993).

[5] H. Benistry, C. M. Sotomayor-Torres, and C. Weisbuch, Phys. Rev. B44, 10945 (1991).

[6] R. W. Morse, J. Acous. Soc. Am. 20, 833 (1948); J. Acous. Soc. Am. 22, 219 (1950).

[7] M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford, London, 1954).

[8] A. A. Maradudin and A: E. Fein, Phys. Rev. 128, 2589 (1962).

[9] P. G. Klemens, Phys. Rev. 148, 845 (1966).

[10] D. K. Ferry, Phys. Rev. B9, 4277 (1974).

[11] P. F. Tua and G. D. Mahan, Phys. Rev. B26, 2208 (1982).

[12] R. Gupta and B. K. Ridley, in *Proceedings of NATO Advanced Research Workshop on Phonons in Nanostructures*, edited by J.-P. Leburton, J. Pascual, and C. Sotomayor Torres (Kluwer, Boston, 1993), pp. 261-272.

[13] P. N. Keating, Phys. Rev. 149, 674 (1966); Phys. Rev. 145, 637 (1966).

[14] Y.-T. Lu and L. J. Sham, Phys. Rev. B40, 5567 (1989).

[15] L. Wendler and R. Haupt, Phys. Stat. Sol. (b) 143, 487 (1987).

[16] G. Gilat and L. J. Raubenheimer, Phys. Rev. 144, 390 (1966).

[17] A. M. de Paula, A. C. Maciel, G. Weber, J. F. Ryan, P. Dawson, and C. T. Foxon, Semicond. Sci. Technol. 7, B120 (1992).

[18] H.-S. Cho and P. R. Prucnal, Phys. Rev. B36, 3237 (1987).

[19] H. C. Liu, Appl. Phys. Lett. 51, 1019 (1987).

3. PERSONNEL

Three faculty members; Dr. K. W. Kim, Dr. G. J. Iafrate, and Dr. M. A. Stroscio, in the Dept. of Electrical and Computer Eng. at North Carolina State Univ. (NCSU) are involved in this research effort. Dr. Kim is currently Associate Professor of Electrical Engineering, and serves as the principal investigator in charge of the day-to-day management and direction of the research program aspects. He is experienced in the Monte Carlo method and other simulation techniques, and has a strong background in theoretical semiconductor physics. His research interests range from the hot electron effects in MOSFETs to quantum transport theory.

Dr. G. J. Iafrate has been engaged in teaching and research for over 20 years, and is currently Adjunct Professor of Electrical Engineering at NCSU and Director of U.S. Army Research Office. His main research interests include solid-state physics and electronics, especially the fundamental questions relating to the breakdown of classical solid-state electronics as device geometries approach the submicron and ultrasubmicron-size regime. Currently, he is involved in the development of a quantum transport formalism to elucidate tunnel-barrier and superlattice hot-electron transport phenomena. Dr. M. A. Stroscio has been associated with NCSU and with U.S. Army Research Office since 1985, most recently as Adjunct Professor of Electrical Engineering and as Senior Research Scientist, respectively. His main research area is quantum transport theory including path integral formalism and solid-state dynamics. He is currently engaged in the study of phonon modes in heterostructures, especially the effects of reduced dimensionality.

Dr. Iafrate and Dr. Stroscio are actively involved in the direction of a post-doctoral associate and a graduate student along with Dr. Kim. Due to the ties with the Army Research Office, the research activities by both Dr. Iafrate and Dr. Stroscio related to this proposal have been at no cost to the Office of Naval Research.

APPENDIX A: List of Refereed Publications on This Program Since 1990

1. K. W. Kim, M. A. Stroscio, and J. C. Hall, "Frequencies of Confined Longitudinal-Optical Phonon Modes in GaAs/GaP Short-Period Strained-Layer Superlattices," *J. Appl. Phys.* 67, 6179 (1990).
2. M. A. Stroscio, K. W. Kim, and J. C. Hall, "Variation in Frequencies of Confined Longitudinal-Optical Phonon Modes due to Changes in the Effective Force Constants near Heterojunction Interfaces," *Superlatt. Microstruct.* 7, 115 (1990).
3. M. A. Stroscio, K. W. Kim, M. A. Littlejohn, and H. Chuang, "Polarization Eigenvectors of Surface-Optical-Phonon Modes in a Rectangular Quantum Wire," *Phys. Rev. B* 42, 1488 (1990).
4. K. W. Kim and M. A. Stroscio, "Electron-Optical-Phonon Interaction in Binary/Ternary Hetero-structures," *J. Appl. Phys.* 68, 6289 (1990).
5. K. W. Kim, M. A. Stroscio, and J. C. Hall, "Frequencies of Confined Longitudinal-Optical Phonon Modes in Short-Period Strained Semiconductor Superlattices," *Proc. SPIE* 1336, 43 (1990).
6. M. A. Stroscio, K. W. Kim, and M. A. Littlejohn, "Theory of Optical-Phonon Interactions in a Rectangular Quantum Wire," *Proc. SPIE* 1362, 566 (1990).
7. M. A. Stroscio, K. W. Kim, and S. Rudin, "Boundary Conditions for Electron-LO-Phonon Interaction in Polar Semiconductor Quantum Wires," *Superlatt. Microstruct.* 10, 55 (1991).
8. K. W. Kim, M. A. Stroscio, A. Bhatt, R. Mickevicius, and V. V. Mitin, "Electron-Optical-Phonon Scattering Rates in a Rectangular Semiconductor Quantum Wire," *J. Appl. Phys.* 70, 319 (1991).
9. M. A. Stroscio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, H. Goronkin, and G. Maracas, "Transition from Longitudinal-Optical Phonon Scattering to Surface-Optical Phonon Scattering in Polar Semiconductor Superlattices," *Appl. Phys. Lett.* 59, 1093 (1991).
10. M. A. Stroscio, K. W. Kim, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Reduction and Control of Inelastic Longitudinal-Optical Phonon Scattering in Nanoscale and Mesoscopic Device Structures," *Proceedings of the 1991 Int. Semiconductor Device Research Symp.*, pp. 87-91, 1991.
11. T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Effects of Finite Hole Lifetime on Electron Transport in P-Type Zincblende Semiconductors," *Proceedings of the 1991 Int. Semiconductor Device Research Symp.*, pp. 235-238, 1991.
12. V. V. Mitin, R. Mickevicius, M. A. Stroscio, G. J. Iafrate, and K. W. Kim, "Electron Dynamics in Quantum Wires," *Proceedings of the 1991 Int. Semiconductor Device Research Symp.*, pp. 111-114, 1991.
13. M. A. Stroscio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, H. L. Grubin, V. V. Mitin, and R. Mickevicius, "Role of Phonon Confinement in Nanoscale Systems," in *Nanostructures and Mesoscopic Systems*, edited by W. P. Kirk and M. A. Reed (Academic Press, San Diego, Calif., 1992), Chap. 8, pp. 379-386.
14. K. W. Kim, M. A. Littlejohn, M. A. Stroscio, and G. J. Iafrate, "Transition from LO-Phonon to SO-Phonon Scattering in Mesoscale Structures," *Semicond. Sci. Technol.* 7, B49 (1992).
15. R. Mickevicius, V. V. Mitin, K. W. Kim, and M. A. Stroscio, "Electron High-Field Transport in Multi-Subband Quantum Wire Structures," *Semicond. Sci. Technol.* 7, B299 (1992).

16. S. Das Sarma, V. B. Campos, M. A. Stroscio, and K. W. Kim, "Confined Phonon Modes and Hot Electron Energy Relaxation in Semiconductor Microstructures," *Semicond. Sci. Technol.* 7, B60 (1992).

17. M. A. Stroscio, K. W. Kim, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Dramatic Reduction of the Longitudinal-Optical Phonon Emission Rate in Polar-Semiconductor Quantum Wires," *Phil. Mag. Lett.* 65, 173 (1992).

18. R. Mickevicius, V. V. Mitin, K. W. Kim, and M. A. Stroscio, "Electron Intersubband Scattering in Real Quantum Wires," *Superlatt. Microstruct.* 11, 277 (1992).

19. R. Mickevicius, V. V. Mitin, K. W. Kim, M. A. Stroscio, and G. J. Iafrate, "Electron Intersubband Scattering by Confined and Localized Phonons in Real Quantum Wires," *J. Phys.: Condens. Matter* 4, 4959 (1992).

20. K. W. Kim, A. R. Bhatt, M. A. Stroscio, P. J. Turley, and S. W. Teitsworth, "Effects of Interface Phonon Scattering in Multi-Heterointerface Structures," *J. Appl. Phys.* 72, 2282 (1992).

21. H. Qiang, F. H. Pollak, C. M. Sotomayor-Torres, W. Leitch, A. H. Kean, M. A. Stroscio, G. J. Iafrate, and K. W. Kim, "Size Dependence of the Electron-Optical Phonon Coupling in GaAs/$Ga_{0.7}Al_{0.3}As$ Single Quantum Wells," *Appl. Phys. Lett.* 61, 1411 (1992).

22. T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Dielectric Response Functions of Highly-Doped Zincblende Semiconductors with Finite Particle Lifetime," *J. Appl. Phys.* 72, 4139 (1992).

23. M. A. Stroscio, K. W. Kim, A. R. Bhatt, G. J. Iafrate, M. Dutta, and H. L. Grubin, "Reduction of Inelastic Longitudinal-Optical Phonon Scattering in Narrow Polar-Semiconductor Quantum Wells," *Proc. SPIE* 1675, 237 (1992).

24. M. A. Stroscio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, A. R. Bhatt, and M. Dutta, "Confined and Interface Optical Phonons in Quantum Wells and Quantum Wires," *Proc. SPIE* CR45, 341 (1993).

25. A. R. Bhatt, K. W. Kim, M. A. Stroscio, G. J. Iafrate, M. Dutta, H. L. Grubin, R. Haque, and X. T. Zhu, "Reduction of Interface Phonon Modes Using Metal-Semiconductor Heterostructures," *J. Appl. Phys.* 73, 2338 (1993).

26. T. Kaneto, K. W. Kim, and M. A. Littlejohn, "Calculation of Minority Carrier Mobilities in Heavily-Doped p-Type Semiconductors in the Dielectric Function Formalism," *Phys. Rev. B* 47, 16257 (1993).

27. M. U. Erdogan, K. W. Kim, and M. A. Stroscio, "Effects of Band Mixing on Hole Tunneling Times in GaAs/AlAs Double-Barrier Heterostructures," *Appl. Phys. Lett.* 62, 1423 (1993).

28. T. Kaneto, K. W. Kim, and M. A. Littlejohn, "A Comparison of Minority Electron Transport in $In_{0.53}Ga_{0.47}As$ and GaAs," *Appl. Phys. Lett.* 63, 48 (1993).

29. M. A. Stroscio, G. J. Iafrate, K. W. Kim, A. R. Bhatt, M. Dutta, and H. L. Grubin, "Reduction in Longitudinal-Optical Phonon Emission Rate in Polar-Semiconductor Quantum Wires and Quantum Wells," in *Phonon Scattering in Condensed Matter VII*, edited by M. Meissner and R. O. Pohl (Springer-Verlag, Berlin, 1993), Springer Series in Solid-State Sciences, Vol. 112, p. 341.

30. M. A. Stroscio and K. W. Kim, "Piezoelectric Scattering of Carriers from Confined Acoustic Modes in Cylindrical Quantum Wires," *Phys. Rev. B* 48, 1936 (1993).

31. M. U. Erdogan, K. W. Kim, M. A. Stroscio, and M. Dutta, "An Extension of Kronig-Penney Model for Γ-X Mixing in Superlattices," *J. Appl. Phys.* 74, 4777 (1993).

32. A. R. Bhatt, K. W. Kim, M. A. Stroscio, and J. M. Higman, "Simplified Microscopic Model for Electron-Optical-Phonon Interactions in Quantum Wells," *Phys. Rev. B* 48, 14671 (1993).

33. M. A. Stroscio, G. J. Iafrate, K. W. Kim, S. Yu, V. Mitin, and N. Bannov, "Scattering of Carriers from Confined Acoustic Modes in Nanostructures," in *Proceedings of the 1993 Intl. Semiconductor Device Research Symp.*, edited by M. Shur and E. Towe (Univ. of Virginia, Charlottesville, Virginia, 1993), pp. 873-875.

34. M. A. Stroscio and K. W. Kim, "Generalized Piezoelectric Scattering Rate for Electrons in a Two-Dimensional Electron Gas," *Solid-State Electron.* 37, 181 (1994).

35. J. He, G. J. Iafrate, and M. A. Littlejohn, "Multi-Band Theory of Bloch Electron Dynamics in Electric Fields," *Semicond. Sci. Technol.* 9, 815 (1994).

36. M. U. Erdogan, V. Sankaran, K. W. Kim, M. A. Stroscio, and G. J. Iafrate, "Real-Space Transfer of Photoexited Electrons in Type-II Superlattices via Optical-Phonon Emission," *Proc. SPIE* 2146, 34 (1994).

37. K. W. Kim, S. Yu, M. U. Erdogan, M. A. Stroscio, and G. J. Iafrate "Acoustic Phonons in Rectangular Quantum Wires: Approximate Compressional Modes and the Corresponding Deformational Potential Interactions," *Proc. SPIE* 2142, 77 (1994).

38. M. U. Erdogan, V. Sankaran, K. W. Kim, M. A. Stroscio, and G. J. Iafrate "Phonon-Assisted Γ-X Transition Rates in Type-II Superlattices," *Phys. Rev. B* 50, 2485 (1994).

39. S. Yu, K. W. Kim, M. A. Stroscio, G. J. Iafrate, and A. Ballato, "Electron-Acoustic-Phonon Scattering Rates in Rectangular Quantum Wires," *Phys. Rev. B* 50, 1733 (1994).

40. M. A. Stroscio, K. W. Kim, S. Yu, and A. Ballato, "Quantized Acoustic Phonon Modes in Quantum Wires and Quantum Dots," accepted for publication in *J. Appl. Phys.*

41. A. R. Bhatt, K. W. Kim, and M. A. Stroscio, "Theoretical Calculation of Longitudinal-Optical Phonon Lifetime in GaAs," accepted for publication in *J. Appl. Phys.*

42. J. He and G. J. Iafrate, "Multi-Band Theory of Bloch Electron Dynamics in a Homogeneous Electric Field," accepted for publication in *Phys. Rev. B.*

43. V. Sankaran, K. W. Kim, and G. J. Iafrate, "Tight-Binding Calculation of Linear Optical Properties of $In_xGa_{1-x}As$ Alloys and Heterostructures," to be published in *Proceedings of the 21th Intl. Symp. on Compound Semiconductors.*

44. J. He and G. J. Iafrate, "Effects of Band-Structure and Electric Fields on Resonant Tunneling Dynamics," to be published in *NATO ASI Series Volume: Quantum Transport in Ultrasmall Devices.*

45. M. U. Erdogan, K. W. Kim, and M. A. Stroscio, "Strain Effects on Hole Tunneling Dynamics in Double Barrier Heterostructures," submitted to *J. Appl. Phys.*

APPENDIX B: Reprints of Publications

This appendix contains the title page of each paper published in the refereed literature which were supported by the ONR project during the 1993-94 contract period. Copies of these papers have been sent to the program manager under separate cover. A list of these papers is included below.

1) M. U. Erdogan, K. W. Kim, M. A. Stroscio, and M. Dutta, "An Extension of Kronig-Penney Model for Γ-X Mixing in Superlattices," *J. Appl. Phys.* 74, 4777 (1993).

2) A. R. Bhatt, K. W. Kim, M. A. Stroscio, and J. M. Higman, "Simplified Microscopic Model for Electron-Optical-Phonon Interactions in Quantum Wells," *Phys. Rev. B* 48, 14671 (1993).

3) M. A. Stroscio, G. J. Iafrate, K. W. Kim, S. Yu, V. Mitin, and N. Bannov, "Scattering of Carriers from Confined Acoustic Modes in Nanostructures," in *Proceedings of the 1993 Intl. Semiconductor Device Research Symp.*, edited by M. Shur and E. Towe (Univ. of Virginia, Charlottesville, Virginia, 1993), pp. 873-875.

4) M. A. Stroscio and K. W. Kim, "Generalized Piezoelectric Scattering Rate for Electrons in a Two-Dimensional Electron Gas," *Solid-State Electron.* 37, 181 (1994).

5) J. He, G. J. Iafrate, and M. A. Littlejohn, "Multi-Band Theory of Bloch Electron Dynamics in Electric Fields," *Semicond. Sci. Technol.* 9, 815 (1994).

6) M. U. Erdogan, V. Sankaran, K. W. Kim, M. A. Stroscio, and G. J. Iafrate, "Real-Space Transfer of Photoexited Electrons in Type-II Superlattices via Optical-Phonon Emission," *Proc. SPIE* 2146, 34 (1994).

7) K. W. Kim, S. Yu, M. U. Erdogan, M. A. Stroscio, and G. J. Iafrate, "Acoustic Phonons in Rectangular Quantum Wires: Approximate Compressional Modes and the Corresponding Deformational Potential Interactions," *Proc. SPIE* 2142, 77 (1994).

8) M. U. Erdogan, V. Sankaran, K. W. Kim, M. A. Stroscio, and G. J. Iafrate "Phonon-Assisted Γ-X Transition Rates in Type-II Superlattices," *Phys. Rev. B* 50, 2485 (1994).

9) S. Yu, K. W. Kim, M. A. Stroscio, G. J. Iafrate, and A. Ballato, "Electron-Acoustic-Phonon Scattering Rates in Rectangular Quantum Wires," *Phys. Rev. B* 50, 1733 (1994).

Extension of the Kronig–Penney model for Γ-X mixing in superlattices

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(Received 30 December 1992; accepted for publication 21 June 1993)

An extension of the Kronig–Penney model to treat mixings of different valleys in superlattices is presented. The value of the mixing parameter α used in the model is deduced by comparison with more sophisticated theory and various experiments for the GaAs/AlAs material system. It is shown that with the use of a single value for the mixing parameter, this simple and efficient model can reasonably reproduce the important aspects of valley mixing effects in GaAs/AlAs superlattices over a wide range of layer thicknesses.

The $GaAs/Al_xGa_{1-x}As$ superlattices with $x>0.43$ have been studied extensively because of their new physical phenomena and possible applications.[1] In these superlattices, for a certain range of layer thicknesses, Γ and X valleys can couple with each other strongly due to the broken translational symmetry of the host lattice caused by the potential discontinuity at the interfaces. Recently, there has been considerable interest in this subject.[2–12] For the conduction bands of superlattices made of direct-gap materials, the Kronig–Penney model can be used satisfactorily. However, other complicated methods[8–11] are required to model the superlattice when this is not the case. An accurate yet simple model for treating mixing effects is useful to make theoretical predictions and explain the experimental results. Therefore, it is very desirable to extend the Kronig–Penney model so that mixings of different valleys may be treated. In this work, we develop such an extension, in which the energy bands and mixed-symmetry wave functions in superlattices are calculated adopting a simplified approach formulated by Cho and Prucnal,[13] along with the boundary conditions introduced by Liu[7] in treating single-barrier tunneling. It is our aim to demonstrate that this simple model with a single value of the mixing parameter for modeling the strength of Γ-X interaction can reproduce the important aspects of the experimental results as well as those of the more complicated theory over a wide range of dimensional scales. This simplified model uses the effective-mass theory, neglects the nonparabolicity effects, and does not deal with lateral mixing due to interface roughness;[11] however, it has the merit of being easy to implement and permits the wave functions to be expressed analytically. Therefore, it can be a valuable tool for simple and efficient calculation of mixing effects.

In a superlattice, the electron state is a mixture of the zone-center Γ and zone-edge X related bulk states. Accordingly, the wave function ψ is written as the sum of the products of slowly varying envelope functions and band-edge periodic functions (Bloch functions): i.e., $\psi=\psi_\Gamma u_\Gamma+\psi_X u_X$, where u_Γ and u_X are the Bloch functions for the Γ and X valleys, respectively. In vector notation, the wave function may be expressed as $\psi=(\psi_\Gamma,\psi_X)$. In a superlattice, the six-fold degeneracy of the X valley is removed, with the formation of an X_z doublet (momentum along the growth axis), and an $X_{x,y}$ quadruplet (momentum in the plane). The $X_{x,y}$ minima are not coupled to the Γ valley due to the conservation of lateral momentum. However, the Γ and X_z valleys are coupled with each other since momentum in the z direction is not conserved because of the discontinuities in the superlattice potential. Accordingly, out of all the X states, only the X_z states are mixed with the Γ states by the perfect superlattice potential, and, herein, the X point will be used to mean X_z particularly. The coupling of Γ and X valleys due to the broken translational symmetry of the crystal can be modeled by the off-diagonal elements in the potential energy.[7] For simplicity, these terms are represented by delta functions centered at the interfaces,

$$V=\begin{pmatrix} V_\Gamma(z) & \alpha\delta(z) \\ \alpha\delta(z) & V_X(z) \end{pmatrix}, \tag{1}$$

where α is a parameter quantifying mixing, $\delta(z)$ is the Dirac delta function, and $V_\Gamma(z)$ and $V_X(z)$ define the Γ-potential discontinuity and X-potential discontinuity, respectively. The wave (envelope)-function continuity condition (at $z=0$) is $(\psi_\Gamma,\psi_X)_{0-}=(\psi_\Gamma,\psi_X)_{0+}$. The other boundary condition can be derived by integration of the Schrödinger equation across the interface,

$$\begin{aligned} -\frac{\hbar^2}{2}\left(\frac{1}{m_\Gamma(z)}\frac{\partial\psi_\Gamma}{\partial z}\bigg|_{0+}-\frac{1}{m_\Gamma(z)}\frac{\partial\psi_\Gamma}{\partial z}\bigg|_{0-}\right)+\alpha\psi_X=0, \\ -\frac{\hbar^2}{2}\left(\frac{1}{m_X(z)}\frac{\partial\psi_X}{\partial z}\bigg|_{0+}-\frac{1}{m_X(z)}\frac{\partial\psi_X}{\partial z}\bigg|_{0-}\right)+\alpha\psi_\Gamma=0. \end{aligned} \tag{2}$$

As can be seen, introduction of the delta-function potential results in a boundary condition in which the Γ and X valleys are coupled across the interface. In obtaining this result, it is assumed that the Bloch functions of the respec-

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Simplified microscopic model for electron–optical-phonon interactions in quantum wells

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A simplified microscopic model of optical phonons in dimensionally confined structures is formulated and applied to calculate electron–optical-phonon scattering rates in GaAs/AlAs quantum wells. For this simplified model which circumvents performing a complicated *ab initio* calculation of the force constants at the interface, it is demonstrated that the resulting dispersion relation and scattering rates for electron–optical-phonon interactions agree very well with those obtained from detailed *ab initio* studies. It is also shown that for GaAs/AlAs structures, the macroscopic dielectric continuum model provides a good approximation to the scattering rate predicted by the microscopic models.

The electronic and optical properties of semiconductor superlattices (SL's) and quantum wells (QW's) have been investigated extensively. A principal advantage of using such heterostructures results from the ability to tailor the electronic and optical properties of the structures for realizing a potentially vast array of high-performance electronic and optoelectronic devices. To fully understand and utilize the properties of these nanometer-scale heterostructures, it is necessary to develop formalisms for studying confinement effects as well as picosecond and subpicosecond processes. It has been known for many years that the scattering by polar–optical-phonon modes is an important energy-loss mechanism for electrons in a wide variety of III-V semiconductor devices. However, effects of confinement on these phonon modes have been investigated extensively only in the past several years.

In recent years, a number of models has been put forward to explain electron–optical-phonon interactions in reduced dimensional systems. They can be broadly classified in two categories: macroscopic[1–9] and microscopic.[10–12] Macroscopic models ignore the effect of individual layers of atoms but they have the considerable advantage of making the interaction calculation very simple. Among these macroscopic models are the dielectric continuum model[1–5] (slab model, which uses purely electrostatic boundary conditions), hydrodynamic model,[7] hybrid model,[8] and a recent dispersive continuum treatment of Nash.[9] In some parameter regimes, these models are fairly accurate and provide good estimates of energy-loss rates. However, scaling of the electron–optical-phonon interaction with diminishing device length presents a serious challenge to the accurate use of such models. As a result, there has recently been an increasing need for more rigorous analysis and detailed knowledge of electron–optical-phonon interactions in reduced dimensional systems. This has been the main motivation for the emergence of *ab initio* microscopic models.[12] Though such models provide the most accurate analysis of the structure, they have not been used extensively. This can be attributed to the fact that the *ab initio* microscopic analysis involves very arduous and time consuming first-principle calculations of lattice dynamics[13,14] rather than employing adjustable parameters.[15–17]

Precise *ab initio* calculations of force constants at the interface may not be essential for most of the heterostructures except those involving extremely thin layers. It is well known that even a simple linear-chain model with nearest-neighbor force constants can predict the zone-center LO-phonon frequencies in a SL with a reasonable accuracy except in the cases where layers are single monolayer thick. Such an approximate model is based on the assumption that atomic-force constants at heterojunction interfaces are identical to those of the bulk or of uniform pseudomorphic layers. In a qualitative analysis of the effect of varying force constants at the heterojunction interfaces of a strained layer, short-period, GaAs/GaP SL with two monolayers per SL layer, it was also found that frequencies of the confined phonon modes are only weakly dependent on the variations in the interfacial force constants.[18] The variation in interfacial force constants by values as extreme as 10% results in less than about a 2% change in the frequencies of confined phonon modes. It should be noted that as a practical matter, changes in the frequencies of the confined LO-phonon modes will be considerably less than 2%, since in most SL's and QW's the ratio of the number of bonds at the interfaces to the number of bonds one or more monolayers away from the interfaces is less than that for the case where each layer is two monolayers thick.

Based on the results of Ref. 18, as well as on supporting observations from other investigators,[19] we have formulated a simplified microscopic model which facilitates the accurate modeling of confined and interface phonons without *ab initio* calculations of force constants. The valence-shell model developed by Kunc and Nielson for bulk[20] has been extended for the SL/QW structures. In-

Proceedings of the 1993 International Semiconductor Device Research Symposium

(Charlottesville, VA, 1993)

Scattering of Carriers from Confined Acoustic Modes in Nanostructures

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Many proposed applications of mesoscopic electronic structures involve carrier transport at low temperatures and low carrier energies; frequently, the regime of interest is one where dimensional confinement modifies the phase space substantially. In this low temperature, low energy regime [1-6], acoustic phonons play an enhanced role in carrier scattering and may dominate over the scattering of carriers by optical phonons. Furthermore, in nanoscale structures it is possible that phase space restrictions may weaken or forbid optical phonon scattering processes that would normally dominate in bulk structures. In recent years, there has been an extensive literature on the role of dimensional confinement in modifying optical phonon modes and their interactions with charge carriers (see, for example, Refs. 7-11 and the numerous papers references therein). However, there are relatively few treatments dealing with the role of dimensional confinement in modifying acoustic phonon modes and their interactions with charge carriers [2-4]. While there is an extensive literature on the theory of acoustic modes in conventional waveguides, resonators and related structures [5], no efforts have been reported to formulate a theory of acoustic phonons in nanoscale structures where both phonon confinement and a quantum mechanical treatment of phonon normalization are both essential; Constantinou has, however, discussed the unnormalized acoustic phonon modes in cylindrical polar semiconductor quantum wires [12].

In recent years, considerable theoretical and experimental effort has focused on understanding the role of confined and interface longitudinal-optical (LO) phonons in nanoscale and mesoscopic semiconductor structures [13]. However, relatively little attention has been given to theoretical treatments of acoustic phonon confinement or to the interaction of confined acoustic phonons with charge carriers. The need for such theoretical treatments has been underscored recently by experimental studies providing both direct and indirect [3,4] evidence of the importance of acoustic phonon confinement in reduced dimensional electronic structures.

In this paper, by appropriately quantizing the acoustic phonon displacements we have obtained the correctly normalized expressions for acoustic phonon confined in a number of dimensionally confined nanostructures. As for the case of LO phonon modes in rectangular quantum wires and quantum dots, there are no exact solutions for the complete set of phonon modes; however, as for the case of LO phonon modes, the approximate modes presented in this work provide simple and useful expressions which are well suited for modeling the interaction of carriers with acoustic phonons. To investigate the effects of reduced dimensionality on the coupling between acoustic phonons and charge carriers, we have formulated the interaction Hamiltonians for both

Solid-State Electronics Vol. 37, No. 1, pp. 181–182, 1994
Printed in Great Britain.

0038-1101/94 $6.00 + 0.00

NOTE

GENERALIZED PIEZOELECTRIC SCATTERING RATE FOR ELECTRONS IN A TWO-DIMENSIONAL ELECTRON GAS

(Received 21 May 1993; in revised form 19 June 1993)

INTRODUCTION

Many envisioned applications of mesoscopic semiconductor structures are based on the transport of charge carriers at low temperatures and at low carrier energies. At such low temperatures and low carrier energies, the scattering of carriers from acoustic phonons may dominate over carrier scattering from optical phonons[1–4]. Transport of carriers in a two-dimensional electron gas is of special importance within the field of carrier transport in semiconductors. In this connection, Price[1] has given an excellent comprehensive treatment of the role of phonon scattering in two-dimensional electron transport in polar semiconductor layers; specifically, for the case of a two-dimensional electron gas, Price has given a detailed account of electron scattering by the Frohlich, deformation and piezoelectric potentials. In the case of piezoelectric scattering of electrons from acoustic phonons, Price has used the piezoelectric constants given by Zook[2] in the form summarized by Hearmon[3]. As discussed by Price, the piezoelectric constants given by Zook were derived under the assumption that the elastic anisotropy of the crystal is small. Price has made the additional approximation of averaging Zook's piezoelectric constants over the azimuthal directions in the plane of the two-dimensional electron gas. In this work, Price's treatment of piezoelectric scattering is generalized by not taking such an average over these azimuthal directions.

DISCUSSION

As discussed previously[1], the piezoelectric scattering rate function, $W(1,2)$, for electrons in a two-dimensional electron gas interacting with the acoustic phonon in a zincblende crystal may be written as:

$$W(1,2)=\frac{2\pi}{\hbar}\frac{S}{(2\pi)^2}2\delta[E(1)-E(2)], \tag{1}$$

where:

$$S=\frac{kT(eh_{14})^2}{2}\frac{\pi}{Q}\left(\frac{B_l}{\rho s_l^2}+\frac{2B_t}{\rho s_t^2}\right), \tag{2}$$

with:

$$B_l=\frac{Q}{\pi}\int_{-\infty}^{+\infty}\frac{A_l}{Q^2+q^2}\,dq, \tag{3a}$$

$$B_t=\frac{Q}{\pi}\int_{-\infty}^{+\infty}\frac{A_t}{Q^2+q^2}\,dq, \tag{3b}$$

$$A_l=36\frac{q^2Q_y^2Q_z^2}{(q^2+Q^2)^3}, \tag{4a}$$

and

$$2A_t+A_l=\frac{4}{(q^2+Q^2)}(q^2Q_y^2+Q_y^2Q_z^2+Q_z^2q^2); \tag{4b}$$

in these results $W(1,2)$ equals the rate of transitions from initial state, 1, to final state, 2, per unit volume of k space, q is the acoustic phonon wavevector normal to a two-dimensional electron gas in the (100) plane, Q_y and Q_z are the phonon wavevectors in the (100) plane, $Q^2=Q_y^2+Q_z^2$, k is Boltzmann's constant, T is the temperature of the lattice, e is the charge on an electron, h_{14} is the piezoelectric constant which has a value of roughly 1.57×10^9 V/m for GaAs, ρ is the mass density, and $s_l(s_t)$ is the longitudinal (transverse) velocity of sound in the lattice. The limitations of eqns (1)–(4b) have been discussed previously in Ref. [1] where it is noted that a linear proportionality between phonon frequency and phonon wavevector has been assumed. Upon performing the indicated integrations over q:

$$\frac{\pi}{Q}B_l=\frac{9}{4}\pi\frac{Q_y^2Q_z^2}{(Q_y^2+Q_z^2)^{5/2}}, \tag{5a}$$

and

$$\frac{\pi}{Q}B_t=\frac{\pi}{2}\frac{1}{(Q_y^2+Q_z^2)^{1/2}}-\frac{3\pi}{4}\frac{Q_y^2Q_z^2}{(Q_y^2+Q_z^2)^{5/2}}. \tag{5b}$$

Thus:

$$S=\frac{kT(eh_{14})^2}{2}\left[\left(\frac{9}{4}\pi\frac{Q_y^2Q_z^2}{(Q_y^2+Q_z^2)^{5/2}}\right)\frac{1}{\rho s_l^2}+\left(\frac{\pi}{2}\frac{1}{(Q_y^2+Q_z^2)^{1/2}}-\frac{3\pi}{4}\frac{Q_y^2Q_z^2}{(Q_y^2+Q_z^2)^{5/2}}\right)\frac{1}{\rho s_t^2}\right]. \tag{6}$$

As in Refs [1–3], the effects of screening have not been considered in deriving eqn (6).

In the limit where the average is taken over azimuthal directions[1]:

$$Q_y^2Q_z^2\to Q^4/8, \tag{7a}$$

and

$$Q_y^2=Q_z^2\to Q^2/2, \tag{7b}$$

with the result that:

$$S=\frac{kT(eh_{14})^2}{2}\frac{\pi}{Q}\left(\frac{9}{32}\frac{1}{\rho s_l^2}+\frac{13}{32}\frac{1}{\rho s_t^2}\right), \tag{8}$$

as originally derived by Price.

In deriving the generalized piezoelectric scattering rate for a two-dimensional electron gas, it has been assumed that the stiffness constants for the zincblende crystal are isotropic. Indeed, for each of GaAs, GaP, InSb, InAs and InP the three independent experimentally-determined stiffness constants differ in magnitude by less than 35% from stiffness constants consistent with an isotropic medium. On the other hand, the generalized expression for $\pi B_l/Q$ may vary from zero to twice its azimuthally averaged value, $9\pi/32Q$ depending upon the relative magnitudes of Q_y and Q_z. While applications such as calculations of mobility were not considered in this work, the fact that the generalized expression for $\pi B_l/Q$ may vanish as Q_y or Q_z goes to zero may be of special significance of the frequently-discussed cases where the dominant charge carrier momentum in the two-dimensional electron gas or the phonon momentum is highly anisotropic; in particular, mobilities for such systems may be enhanced since the longitudinal scattering terms may be suppressed as a result of the anisotropic form of eqn (5a). The variation in $\pi B_l/Q$ is much less pronounced having a range from $10\pi/32Q$ to $16\pi/32Q$ depending upon the relative magnitudes of Q_y and Q_z.

Semicond. Sci. Technol. 9 (1994) 815–819. Printed in the UK

Multiband theory of Bloch electron dynamics in electric fields

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Abstract. A novel multiband theory of Bloch electron dynamics in homogeneous electric fields of arbitrary strength and time dependence is presented. In this formalism, the electric field is described through the use of the vector potential. Multiband coupling is treated through the use of the Wigner–Weisskopf approximation, thus allowing for a Bloch electron transition out of the initial band due to the power absorbed by the electric field; also, the approximation ensures conservation of the total transition probability over the complete set of excited bands. The choice of the vector potential gauge leads to a natural set of extended time-dependent basis functions for describing Bloch electron dynamics in a homogeneous electric field; an associated basis set of localized, electric-field-dependent Wannier and related envelope functions are developed and utilized in the analysis to demonstrate the inherent localization manifest in Bloch dynamics in the presence of relatively strong electric fields. From the theory, a generalized Zener tunnelling time is derived in terms of the applied uniform electric field and the relevant band parameters. The analysis shows an electric-field-enhanced broadening of the excited state probability amplitudes, thus resulting in spatial lattice delocalization and the onset of smearing of discrete, Stark ladder and band-to-band transitions due to the presence of the electric field. In addition, the velocities of a Bloch oscillation will be observed only for the electron that is initially in a Bloch state before Zener tunnelling. Further, the influence of electric fields on resonant tunnelling structure is examined.

1. Introduction

Bloch electron dynamics in a homogeneous electric field has been a subject of great interest dating back to the earliest applications of quantum mechanics to solid state physics [1–3]. Even more recently, as modern fabrication technologies continue to drive the study of solid state transport into the nanometre domain, many new and interesting questions have emerged concerning the solid state dynamics and quantum transport of carriers in 'band-engineered' superlattices and tailored periodic solids.

In this paper, a novel multiband theory of Bloch electron dynamics in homogeneous electric fields of arbitrary strength is presented. In this formalism, the electric field is described through the use of the vector potential; in this regard, this work builds on the methodology previously developed by one of the authors (GJI) and co-workers [1–3] to describe solid state dynamics and quantum transport for Bloch electrons in an applied homogeneous electric field of arbitrary strength and time dependence, including weak scattering from randomly distributed impurities and phonons [1], and a spatially localized, inhomogeneous electric field [3]. In addition, multiband coupling is treated in the Wigner–Weisskopf (W–W) [4] approximation, a classic approach for describing the time decay from an occupied quasistationary state; the W–W approximation allows for the analysis of the long-time, time-dependent tunnelling characteristics of an electron transition out of an initially occupied band due to the power absorbed by the electric field, while preserving conservation of total transition probability over the complete set of excited bands.

The choice of the vector potential gauge leads to a natural set of basis functions for describing Bloch electron dynamics in a homogeneous electric field. A basis set of localized, electric-field-dependent Wannier functions and associated envelope equations are developed to accommodate the inherent localization manifest in Bloch dynamics due to a relatively strong electric field.

Building on previous methodology [3], use is made of the instantaneous eigenstates of the Hamiltonian describing a Bloch electron in an electric field

$$H = \frac{1}{2m}\left(P - \frac{e}{c}A_0(t)\right)^2 + V_c(x) \qquad (1)$$

where $V_c(x)$ is crystal potential, $A_0 = -cE_0t$ is the vector potential for the time-independent homogeneous electric field, E_0, turned on at initial time $t = 0$. The solution

0268-1242/94/050815-05$19.50

Real-space transfer of photoexcited electrons in type-II superlattices via optical-phonon emission

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ABSTRACT

The Γ-X scattering rate of electrons in type-II superlattices by optical-phonon emission is calculated. The tight binding method for electronic band structure and the dielectric continuum model for phonons are used. The relative strength of scattering due to different phonon modes is examined for varying superlattice dimensions. The scattering rate is highest when the energy separation between the Γ and X levels is smallest, and decreases quickly as the separation increases. It is found that the strongest scattering rate is due to the emission of AlAs confined modes. Changing of parity with layer thickness and its effect on scattering are discussed.

1. INTRODUCTION

Recently, there has been considerable interest in hot carrier dynamics in heterostructures. One important issue in this area has been the relaxation of photoexcited carriers in heterostructures from higher energy subbands to the lower ones. This process has been studied extensively both experimentally and theoretically because of its fundamental physics and for possible device applications.[1-6] Most of the work up to now has been on type-I heterostructures where the bandgap of one material is entirely nested within the gap of another material. In this structure, electrons and holes are both localised in the same layer. On the other hand, in the so-called type-II superlattices, the holes are localised in one layer, whereas the lowest energy electrons are contained in the other layer.[7] The well studied $Al_xGa_{1-x}As/GaAs$ superlattices can be made type-II by appropriately choosing the layer thicknesses and alloy composition. For example, the GaAs/AlAs superlattices with thick AlAs layers are known to be type-II for GaAs layer thicknesses less than or equal to 35 $\AA$ (12 monolayers).[7] Type-I to type-II transitions can also be achieved by application of external forces such as an electric field or hydrostatic pressure. In the case of type-II structures, the lowest conduction band level is not in the GaAs but in the $Al_xGa_{1-x}As$ layer. In type-I heterostructures, electrons photoexcited from the valence band to the conduction band relax to lower energy levels within the same layer. However, in type-II structures, the electrons excited to a direct-gap energy level (Γ) in one layer then can relax to an indirect-gap energy level (X) in the adjacent layer. This is a very interesting case because electron relaxation happens with real-space transfer. This

0-8194-1441-7/94/$6.00

Acoustic phonons in rectangular quantum wires: approximate compressional modes and the corresponding deformation potential interactions

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ABSTRACT

The Hamiltonian describing the deformation potential interaction of confined acoustic phonons with carriers is derived by quantizing the appropriate, experimentally-verified approximate compressional acoustic phonon modes in a rectangular quantum wire. The scattering rate due to the deformation potential interaction is calculated for a range of quantum wire dimensions.

1. INTRODUCTION

Many proposed applications of mesoscopic electronic structures involve carrier transport at low temperatures and low carrier energies; frequently, the regime of interest is one where dimensional confinement modifies the phase space substantially. In this low temperature, low energy regime,[1-6] acoustic phonons play an enhanced role in carrier scattering and may dominate over the scattering of carriers by optical phonons. Furthermore, in nanoscale structures it is possible that phase space restrictions may weaken or forbid optical phonon scattering processes that would normally dominate in bulk structures. In recent years, there has been an extensive literature on the role of dimensional confinement in modifying longitudinal optical (LO) phonon modes and their interactions with charge carriers in nanoscale and mesoscopic semiconductor structures (see, for example, Refs. 7-12 and the numerous papers referenced therein). However, there are relatively few treatments dealing with the role of dimensional confinement in modifying acoustic phonon modes and their interactions with charge carriers.[2-4] While there is an extensive literature on the theory of acoustic modes in conventional waveguides, resonators and related structures, few efforts have been reported to formulate a theory of acoustic phonons in nanoscale structures where both phonon confinement and a quantum mechanical treatment of phonon normalization are essential; Constantinou has, however, discussed the unnormalized acoustic phonon modes in a cylindrical polar semiconductor quantum wire.[13] The need for such theoretical treatments has been underscored recently by experimental studies providing both direct and indirect[3,4] evidence of the importance of acoustic phonon confinement in reduced dimensional electronic structures.

0-8194-1437-9/94/$6.00

Phonon-assisted Γ-X transition rates in type-II superlattices

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(Received 7 March 1994)

The Γ-X transition rate for electrons in type-II superlattices is calculated for the case of optical-phonon emission. The tight-binding method for electronic band structure and the dielectric continuum model for phonons are used. The relative strength of scattering due to different phonon modes is examined for varying superlattice dimensions. The scattering rate is highest when the energy separation between the Γ and X levels is smallest, and decreases quickly as the separation increases. It is found that the strongest scattering rate is due to the emission of AlAs confined modes. Changing of parity with layer thickness and its effect on scattering are discussed.

I. INTRODUCTION

Recently, there has been considerable interest in hot-carrier dynamics in heterostructures. One important issue in this area has been the relaxation of photoexcited carriers from higher-energy subbands to the lower ones. This process has been studied extensively both experimentally and theoretically because of its fundamental nature as well as for possible device applications.[1-7] Most of the work up to now has been on type-I heterostructures where the band gap of one material is entirely nested within the band gap of another material. Consequently, electrons and holes are both localized in the same layer in these structures. On the other hand, in the so-called type-II superlattices, the holes are localized in one layer, whereas the lowest-energy electrons are contained in the opposite layer.[8] This is due to the staggered band alignment in these heterostructures. The well-studied $Al_xGa_{1-x}As/GaAs$ superlattices can be made type-II by appropriately choosing the layer thicknesses and alloy compositions. For example, GaAs/AlAs superlattices with thick AlAs layers are known to be type-II for GaAs layer thicknesses less than or equal to 35 Å (12 monolayers).[8] Type-I to type-II transitions can also be achieved by application of external forces such as an electric field or hydrostatic pressure. In the case of type-II structures, the lowest conduction-band level is not in the GaAs but in the $Al_xGa_{1-x}As$ layer. In type-I heterostructures, electrons photoexcited from the valence band to the conduction band relax to lower-energy levels within the same layer. However, in type-II structures, the electrons excited to a direct-gap energy level (Γ) in one layer then can relax to an indirect-gap energy level (X) in the adjacent layer. This is a very interesting case because electron relaxation occurs in conjunction with real-space transfer. This process, which is normally forbidden, is now possible due to the mixing of Γ and X states by the superlattice potential and relaxation of momentum conservation due to interface disorder (lateral mixing). Several experimental results related to Γ-X transfer are available in the literature.[5-7] In spite of the spatial charge transfer, the relaxation rate can be very high. Experimental evidence has been presented that Γ-X electron transfer occurs by the emission of long-wavelength optical phonons.[7] However, a detailed theoretical analysis for the Γ-X transfer in type-II structures has not yet been given.

In this paper, we calculate the Γ-X scattering rates due to optical-phonon emission using a realistic band-structure model and show that this is an important mechanism for the Γ-X relaxation process in type-II superlattices. The paper is organized as follows. In Sec. II, we present the tight-binding model and the dielectric continuum model used in the calculation. Evaluation of matrix elements is explained. In Sec. III, we present and discuss our results of electron relaxation rates. Finally, in Sec. IV, a summary is given.

II. FORMULATION

It is well known that the electron–optical-phonon interaction in low-dimensional systems can be altered strongly due to the confinement of the carriers and the confinement of the phonons. Usually, a single-band, spherical effective-mass model is used for the description of the confined carrier states. It is commonly assumed that each of these states is derived from bulk states of a given symmetry only (e.g., Γ, X, or L), and levels derived from different bulk states do not interact with each other. In a superlattice, momentum in the growth direction is not conserved due to the discontinuities in the superlattice potential in this direction. Therefore, bulk states of the same energy but different symmetry can couple with each other. For a superlattice grown in the z direction, the sixfold degeneracy of the X valley is removed, with the formation of an X_z doublet having momentum along the growth axis, and an $X_{x,y}$ quadruplet, with momentum in the plane. The $X_{x,y}$ and L minima are not coupled to the Γ valley due to the conservation of lateral momentum. Therefore, only the Γ and X_z valleys are coupled

Electron–acoustic-phonon scattering rates in rectangular quantum wires

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Electron–acoustic-phonon scattering in a rectangular quantum wire is studied. The Hamiltonian describing the deformation-potential interaction of confined acoustic phonons with carriers is derived by quantizing the appropriate, experimentally verified approximate compressional acoustic-phonon modes in a free-standing rectangular quantum wire. The scattering rate due to the deformation-potential interaction is obtained for GaAs quantum wires with a range of cross-sectional dimensions. The results demonstrate that a proper treatment of confined acoustic phonons may be essential to correctly model electron scattering rates at low energies in nanoscale structures.

I. INTRODUCTION

A number of proposed applications of mesoscopic electronic structures involve carrier transport at low temperatures and low carrier energies; frequently, the regime of interest is one where dimensional confinement modifies the phase space substantially. It is well known that in this low-temperature, low-energy regime,[1–6] acoustic phonons play an enhanced role in carrier scattering and may dominate over the scattering of carriers by optical phonons. In addition, in nanoscale structures it is possible that phase-space restrictions may weaken or forbid optical-phonon scattering processes that would normally dominate in bulk structures. Recently, there has been an extensive literature on the role of dimensional confinement in modifying longitudinal-optical (LO) phonon modes and their interactions with charge carriers in nanoscale and mesoscopic semiconductor structures (see, for example, Refs. 7–12 and the numerous papers referenced therein). On the other hand, there are relatively few treatments dealing with the role of dimensional confinement in modifying acoustic-phonon modes and their interactions with charge carriers.[2–4,13,14] In spite of the fact that there is an extensive literature on the theory of acoustic modes in conventional waveguides, resonators, and related structures, few efforts have been reported on formulating a theory of acoustic phonons in nanoscale structures, where both phonon confinement and a quantum-mechanical treatment of phonon normalization are essential. The necessity for such theoretical treatments has been demonstrated recently by experimental studies providing both direct and indirect[3,4] evidence of the importance of acoustic-phonon confinement in reduced dimensional electronic structures.

In this paper, we have obtained the normalized expressions for acoustic phonons confined in a free-standing rectangular quantum wire by appropriately quantizing the acoustic-phonon displacements. As is well known, there are no exact solutions for the complete set of phonon modes for a rectangular quantum wire; nevertheless, as for the case of LO phonon modes,[8] the approximate modes presented in this work provide simple and useful expressions, which are well suited for modeling the interaction of carriers with acoustic phonons. As a basis for investigating the role of reduced dimensionality on the coupling between acoustic phonons and carriers, we have formulated the interaction Hamiltonian for the deformation potential associated with confined acoustic-phonon modes in rectangular quantum wires. The resulting scattering rates (based on the golden rule approximation) are compared with those obtained from the bulk-phonon modes. For numerical calculations, GaAs is used as the material of choice throughout this study.

II. QUANTIZATION OF COMPRESSIONAL ACOUSTIC-PHONON MODES FOR A RECTANGULAR QUANTUM WIRE

The compressional, or dilatational, acoustic-phonon modes in free-standing rods of rectangular cross section have been examined both experimentally[15] and theoretically[16,17] by Morse in an extended study. Morse has derived an approximate set of hybrid compressional, or dilatational, acoustic-phonon modes,[16,17] which are found to accurately approximate the experimentally observed modes over a wide range of conditions.[15] Specifically, Morse has found that the approximate hybrid modes derived by assuming separable boundary conditions[16,17] have simple analytical representations and provide convenient approximations for the rectangular geometry when the cross-sectional dimensions have aspect ratios of approximately 2 or greater. For smaller aspect ratios (i.e., close to 1), Morse has argued correctly that it is necessary to turn to numerical solutions since exact

